MODELLING AND SIMULATION OF DEEP BED FILTERS FOR WATER CLARIFICATION

A Thesis Submitted in Partial Fulfilment of the Requirements for the Degree of

DOCTOR OF PHILOSOPHY

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By VINOD TARE

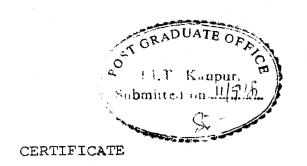
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C. Venkobachar

C. Venkobachar

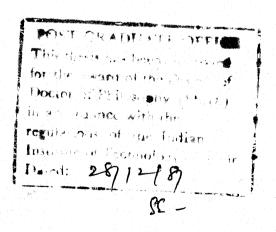
Assistant Professor

Environmental Engineering Division

Department of Civil Engineering

Indian Institute of Technology

KANPUR



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LIST OF SYMBOLS

```
a
               = coefficient of filtration rate expression, Eq. (2.9);
               = collector radius;
ac
\mathtt{a}_\mathtt{i}
               = exponent of pressure gradient equation, Eq. (2.23);
               = suspended particle radius;
ap
A
               = area of the filter bed;
A1,A2,A3
               = empirical constants given by Eq. (6.12);
Ac
               = surface area of filter grains;
A
               = quantity defined by Eq. (2.19);
b
               = radius of the outer shell of the sphere-in-cell
                 model:
               = volume concentration of particulate matter in
C
                  liquid;
               = \eta \alpha v_0 \frac{\pi}{4} d_C^2;
C
              = \eta_{p} \alpha_{p} v_{p} \frac{\pi}{4} d_{p}^{2};
               = \eta/\eta_p C_2 \beta_c + (1 - \beta_c)C_2;
 C_{2}
               = c_2 \beta_p;
 C_{4}
d<sub>c</sub>
               = diameter of the media grain;
               = grain diameter;
ďa
               = suspended particle diameter;
d<sub>p</sub>
               = particle diffusion coefficient in liquid;
D_{BM}
e_{1}, e_{2}, e_{3}, e_{4} = exponents of Eq. (2.10);
               = function describing the effect of particle
 f(\alpha', \sigma)
                  deposition on filter coefficient;
               = porosity of the filter bed;
 F
               = porosity of clean filter bed;
 Fo
```

```
F_1(\beta, \sigma) and = functions describing the effect of particle
                deposition on pressure gradient;
F_{2}(\beta, \sigma)
Fa
              = porosity of deposits;
              = porosity in the jth time interval;
Fi
g
              = acceleration due to gravity;
G(\gamma, c, \sigma)
              = function expression for filtration rate;
GM
              = geometric mean size;
hf
              = head loss at any time t;
              = head loss in clean bed;
hfo
Η
              = Hamaker's constant;
k
              = Boltzmann's constant;
K '
              = empirical constant;
              = depth of the filter bed;
L
              = number of particle sizes;
m
m_1
              = a constant;
Μ
              = number of terms of the pressure gradient equation,
                Eq. (2.23);
              = local particle concentration;
n
no
              = influent particle concentration;
              = effluent particle concentration in j tn time
n<sub>e</sub>i
                interval;
              = influent particle concentration in j th time
                interval;
              = number of retained particles acting as collectors;
Ν
              = number of filter grains in the unit volume of the
NC
                bed:
              = number of retained particles in the unit volume of
                the bed;
              = total number of length elements;
NL
              = total number of time intervals;
NT
              = pressure;
p
```

```
p_i
                = coefficient of Eq. (2.23);
  P
                = quantity defined by Eq. (2.20);
 P_1
               = coefficient of Eq. (2.10);
 Рe
                = Peclet number given by Eq. (6.7);
  R
               = coefficient of correlation;
- S.
               = standard error of estimate;
  t
               = time;
  T
               = absolute temperature;
 u
               = superficial velocity of filter bed;
  \mathbf{v}_{_{\Omega}}
               = approach velocity or superficial velocity;
  V_{\infty}
               = interstitial velocity of filter bed;
               = volume of filter grains;
               = quantity defined by Eq. (2.21);
               = Ln (polymer dose, mg/lit.);
  Х
               = parameter vector in Eq. (2.7);
 X
  \mathbf{z}
               = axial distance;
               = particle-to-filter grain attachment coefficient;
  \alpha_1, \alpha_2, \alpha_3 = exponents of Eq. (2.8);
               = particle-to-particle attachment coefficient;
 α
               = parameter vector of function f_{i}(\alpha', \sigma);
               = parameter vector of functions F_1(\beta, \sigma) and
 β
                  \mathbf{F}_{2}(\beta, \sigma);
               = components of \beta;
  β1. β2
               = fraction of the retained particles acting as
  \beta_{c}
                  collectors contributing for the reduction in
                  effective area of the media grain;
               = fraction of the retained particles which contri-
                  bute for the reduction in effective surface area
                  of the retained particles acting as collectors;
```

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```
β¹
             = portion of the retained particles which contribute
                to the additional surface area;
β"
             = fraction of the removed particles acting as
                collectors;
             = parameter vector of function G(\gamma, c, \sigma);
γ
ΔFj
             = change in porosity in the J+1<sup>th</sup> time interval
                compared to the initial porosity;
ΔL
             = thickness of the Unit Bed Element;
             = surface potentials of particle and grain;
Ψ01* Ψ02
η
             = collision efficiency of clean media;
η<sub>c</sub>
             = single collector collision efficiency;
\eta_{\mathbf{D}}
             = single collector collision efficiency due to
                Brownian diffusion;
\boldsymbol{\eta}_{G}
             = single collector collision efficiency due to
                sedimentation;
\dot{\eta}_{\mathtt{I}}
              = single collector collision efficiency due to
                interception;
              = particle-to-particle collision efficiency;
\eta_{\mathbf{P}}
^{\eta}r
              = single collector removal efficiency;
n :
              = collection efficiency of collector;
              = corrected time defined by Eq. (2.3);
0
K
              = double-layer reciprocal thickness;
λ
              = filter coefficient;
10
              = clean filter coefficient;
λ<sub>e</sub>
              = wavelength of electron oscillation;
              = viscosity;
μ
              = density of liquid;
ρ
              = density of suspended particles;
              = specific deposit (volume of deposited matter per
σ
                unit volume of bed);
              = ultimate specific deposit;
 max
```

SYNOPSIS

Vinod Tare
Ph.D.
Indian Institute of Technology, Kanpur
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MODELLING AND SIMULATION OF DEEP BED FILTERS FOR WATER CLARIFICATION

Filtration is a subject which has, in recent years, developed a rich and varied literature. Despite the dramatic progress in understanding filtration process, a comprehensive method capable of predicting the dynamic behaviour of a filter over its entire operational span has remained out of reach. No doubt, the uncertainties of the nature of the deposition process, particularly the critical ones relating to the nature of the distribution of the deposited matter within the media and its evolution with progressive deposition, have stood as the main impediments obstructing progress towards such a general predictive scheme. In the present research this problem is resolved by postulating an overall picture of the filtration process which incorporates the significant role played by the retained particles on filter performance as the filtration progresses.

The ultimate objective of the theoretical approach is to derive mathematical formulations which quantitatively describe the compllete dynamics of deep bed filtration, taking into account the compllexed interaction between the filter grains and liquid solution particles to be removed as well as the effects of

operating and system variables. At this stage of its development, it has been possible to predict with reasonable accuracy the head loss and efficiency of clean filters. During filtration, both head loss and removal efficiency change with time. These changes are caused by particles that are retained in the filter bed. the present research an attempt has been made to formulate a new conceptual model for predicting the filter performance as the filtration progresses based on the concept that the filtration of suspended particles in deep bed filters is a two stage process. The first stage involves the transport of suspended particles to the media grain or already deposited particles and the second stage accounts for the attachment of these particles to the media grain or the deposited particles. It is postulated that the deposited particles act as collectors, and some fraction of the deposited particles contribute for the reduction in effective area of the media grain and retained particles acting as collectors.

To provide a physically realistic model as basis for quantitative descriptions of the various processes of interest which occur in the porous medium, the concept of Unit Bed Element (UBE) and of the unit collector is used. The filter bed is postulated to consist of a number of unit bed elements in series. Each one in turn is assumed to consist of a number of single collectors. The capacity of the bed to remove particulate matter can be described by the collection efficiency of the unit bed element, defined as the fraction of suspended particles entering the UBE removed.

At the first stage of model development, the filtration efficiency is described by a set of three interdependent equations for monosized particles in suspension assuming the porosity of the bed to remain constant as the filtration progresses. The first equation computes the single collector efficiency related to clean grain efficiency and retained particles acting as collectors. The second equation estimates the number of retained particles acting as collectors as a function of depth, time and local particle concentration in suspension. The third equation predicts suspended particle concentration with time over the entire filter depth. The head loss development is predicted by modifying the classical head loss equation for clean filters incorporating change in the surface area to volume ratio of the filter grains.

In the second stage, the model is refined to eliminate and check the assumption of constant porosity. The change in porosity is computed from the decreased pore volume because of the retained particles. Finally, the model is extended to include the effect of multisized particles in suspension as well as the multisized media.

The model is verified with a set of laboratory data obtained from literature and the experimental investigation carried out during the present research. Uniform latex particles with mean diameters of 0.109, 1.1 and 7.6 microns were used as the turbidity in the filter influent in most of the experiments. Appropriate experiments were conducted in which the size and concentration of suspended particles were varied while physical and hydraulic filtration parameters were maintained at constant levels. The

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model predicted values very well agree with almost all experimental observations.

The simulation of deep bed filters is achieved in two steps. The first step involves the simulation of filter performance characterized by the effluent quality and head loss development. The second step includes the simulation of filter state characterized by the clogging zone. The clogging zone is obtained by proposing an equation for the clogging front. The filter performance and filter state are simulated for various physical and physico-chemical parameters influencing water and wastewater filtration such as size, density and concentration of suspended particles, size of the media, initial bed porosity, flow rate, particle-to-media grain attachment, and particle-to-particle attachment by experimenting on the proposed model. The model is able to predict the filter performance in accordance with the observations made in laboratory and field.

1. INTRODUCTION

Filtration, a physico-chemical process is one of the most important unit operations employed for the final clarification of water and wastewater in treatment plants. The process involves the retention of suspended and colloidal particles by the filter grains and/or previously retained particles as the suspension is made to pass through the granular filter bed. The main indicators of the dynamic behavior of the operation are filtrate quality history and the pressure drop history required to maintain a uniform throughput. The first defines the effectiveness and the capacity of the filter bed, and the second determines the length of the filter run.

The importance of an accurate simulation of the dynamics of packed bed filtration is evident, as it provides the basis for rational design and optimization. Recent advances in the study of deep bed filtration have shown that inspite of the inherent complexities of the process, the problem can be studied fruitfully based on fundamental consideration. Resurgent research efforts of the past two decades in this relatively old engineering practice have already yielded important results of practical significance. In general, the study of deep bed filtration has been made using two different yet often complementary approaches: phenomenological and theoretical. The phenomenological approach describes

the dynamic behavior of deep bed filters with the use of a set of partial differential equations and characterizes the filtration mechanisms by means of several model parameters the values of which, for a given application, can be obtained from appropriate bench scale experiments. The solution of these equations provides the basis of design, scale up and optimization. Although this approach affords only limited insight about the physical process of filtration and is therefore not entirely satisfactory from scientific viewpoints, it represents a practical and rational methodology to the design of industrial scale depth filters, provided the bench scale experiments from which the relevent parameters are obtained can be conducted with sufficient accuracy.

The ultimate objective of the second approach viz., theoretical, is to derive mathematical formulations which quantitatively describe the complete dynamics of deep bed filtration, taking into account the complexed interaction between the filter grains and liquid solution particles to be removed as well as the effects of operating and system variables. At this stage it has been possible to predict with reasonable accuracy the performance of clean bed filters in terms of head loss development and removal efficiency. The loss of head at the start of filtration can be predicted by knowing the media size, filtration rate, and bed porosity. Similarly, the removal efficiency of clean bed filters depends on the characteristics of suspended particles and

filter media like size, density and surface properties, the filtration velocity and the depth and porosity of the filter bed.

During filtration, both head loss and removal efficiency change with time. These changes are caused by particles that are retained in the filter bed. O'Melia and Ali (1978) proposed a model for the development of head loss and removal efficiency during filtration by packed beds based on the postulate that some retained particles can act as collectors and thereby improve filtration efficiency. Though, the concept seems to be appropriate and the mathematical model agrees within the certain limits of experimental data, the estimated coefficients may not reflect or may not have any correlation with the actual properties of the suspension and filter media responsible for filtration. This is because the aforementioned model fails to properly incorporate few important factors, such as surface coverage of the filter media grains and that of retained particles acting as collectors, variation of retained particles acting as collectors along the filter depth etc., which would influence the filter performance to a large extent.

Therefore the present research was undertaken with the main objective to formulate a new conceptual model incorporating above-mentioned factors which would help in dynamic simulation of filter performance. The model should be able to predict the filter performance in accordance with the

observations made in laboratory and field. Using the proposed model an equation is developed for the depth of floc penetration which would help in evaluating the optimum filter depth.

2. LITERATURE REVIEW

Filtration of water through a porous media is an old process in the field of water purification. Slow sand filters were introduced in Scotland in 1804 and into the United States in 1872 (Fuller, 1933). Rapid sand filters came into existence towards the end of the nineteenth century and since then it has become a major unit operation in water purification plants. The main function of rapid sand filtration is the final clarification of settled water. Many attempts have been made to enhance this achievement in order to cope with demands for larger amounts of higher quality water. Thus a considerable interest in the practice and theory of water filtration has been maintained. Early developments were focused on refining the structural features of filter; this was followed by a period of refinement in filter operation. Subsequently, emphasis was placed on proper conditioning of the water prior to the filtration. In recent decades attention has been directed towards the understanding of the mechanisms of the filtration process so that additional improvements and innovations can be obtained.

This continuous interest on the subject of water filteration has generated a rather extensive literature. This literature is so broad that a comprehensive review of all these publications would be quite lengthy and beyond the scope of this dissertation. Furthermore, such reviews are

available elsewhere (Agrawal, 1966; Habibian, 1971; Ali, 1977; Tien and Payatakes, 1979). However, to facilitate the discussion of the scope and results of this thesis, a summary of pertinent literature is presented here.

In general, the study of deep bed filtration has been made using two different yet often complementary approaches: phenomenological and theoretical. The phenomenological approach views the filtration process at macroscopic level and is aimed at (1) predicting the dynamic behavior of filtration process; (2) development of methodology and technique for design, calculation, and optimization. The theoretical approach studies the deep bed filtration at microscopic level and is intended to provide information and insight about the mechanisms of particle deposition, the conditions under which this occurs, and the effect of deposition on the structure and characteristics of filter grains.

2.1 Phenomenological Approach

2.1.1 Prediction of Filtrate Quality

The fundamental equations describing the particle retention of a filter bed are the macroscopic conservation equation and the rate equation. The conservation equation is similar to that used in any fixed bed process involving the transport of matter from the mobile to the stationary phase. For an axial flow filter with a constant cross-sectional area, this is written as

$$u(\frac{\partial c}{\partial z})_{t} + \left[\frac{\partial (\sigma + Fc)}{\partial t}\right]_{z} = 0$$
 (2.1)

Here, u is the superficial velocity, c is the volume concentration of particulate matter in liquid, z is the axial distance, t is the time, σ is the specific deposit, and F is the porosity of filter bed.

The assumptions involved are one dimensional plug flow and negligible axial dispersion of particulates. The porosity of the bed F changes with time as particle accumulation within the bed increases. If the deposited matter forms relatively smooth coating on the external surface of the filter grains, F and σ can be related by the simple expression

$$F = F_0 - \frac{\sigma}{1 - F_d} \tag{2.2}$$

Here, \mathbf{F}_{o} is the porosity of clean bed and \mathbf{F}_{d} is the porosity of deposits.

On the other hand, if the deposit morphology is largely of the blocking type, a different expression relating F, σ , and the interstitial velocity results.

Similar to all fixed bed processes, it is more meaningful to employ a corrected time variable @ defined as

$$e = t - \int_{0}^{z} \frac{F}{u} dz \qquad (2.3)$$

In terms of the variables (z, 0), Eq. (2.1) becomes

$$\mathbf{u}(\frac{\partial \mathbf{C}}{\partial \mathbf{z}})_{\Theta} + (-\frac{\partial \mathbf{Q}}{\partial \Theta})_{\mathbf{z}} = 0$$
 (2.4)

The difference between t and 0 is usually small. However, it may become important in the interpretation of data from small experimental filters.

To complete the description, the rate expression of filtration needs to be specified. In general, this can be expressed as

$$\left(\frac{\partial \sigma}{\partial \Theta}\right)_{z} = -u\left(\frac{\partial C}{\partial z}\right)_{\Theta} = G(\gamma, C, \sigma) \tag{2.5}$$

Here, γ is the parameter vector of function $G(\gamma$, c, σ).

Based on slow sand filter data, Iwasaki (1937) proposed the expression

$$= \left(\frac{\partial C}{\partial z}\right)_{t} = \lambda C \qquad (2.6a)$$

Here, λ is the filter coefficient.

If one ignores the difference between t and θ , combining Eqs.(2.5) and (2.6a) yields

$$\left(\frac{\partial \sigma}{\partial \Theta}\right)_{Z} = u \lambda c \qquad (2.6b)$$

In other words, use of Iwasaki's assumption is tantamount to the use of a first-order expression for the rate of filtration. Later, Ives (1960) applied Eq. (2.6a) to rapid sand filters successfully. The validity of this expression was also shown experimentally by Ison and Ives (1969).

From physical considerations one would expect λ to be a function of the state of the media. This is confirmed

by experimental observations. To account for the variation of λ due to particle accumulation in the bed, one may write

$$\lambda = \lambda_0(X) f_{\lambda}(\alpha^{t}, \sigma)$$
 (2.7)

with

$$f_{\lambda}(\alpha',0) = 1$$

Here, $\lambda_{_{\rm O}}$ is the value of λ when the bed is clean, X is the parameter vector (including quantities such as interstitial velocity, grain size, density difference, etc.) on which $\lambda_{_{\rm O}}$ depends, and f_{λ} (α ', σ) is the function describing the effect of particle deposition on filter coefficient.

The empirical determination of the functional form of f_{λ} (α' , σ) from experimental data has been attempted by a number of investigators. Extensive reviews on this can be found in Agrawal (1966), Ives (1969, 1971), and Herzig et.al. (1970). Table 2.1 lists some of the expressions proposed. Generally speaking, most of the proposed expressions can be derived from a general equation proposed by Ives (1967, 1969) and Mohanka (1969).

$$f_{\lambda} = (1 + 1 - F_{o})^{\alpha_{1}} (1 - F_{o})^{\alpha_{2}} (1 - F_{o})^{\alpha_{3}}$$
 (2.8)

Here, α_1 , α_2 , α_3 are empirical constants, and σ_{\max} is the maximum value of σ to be achieved in filtration.

It is implicitly assumed that filter media will ultimately become nonretentive owing to the change of surface characteristics, increased reentrainment, etc.

Table 2.1. Some analytical solutions of filtration equations (Adopted from Tien and Payatakes, 1979)

s. No.	Investigator	Rate expression	Solution for filtrate quality
1	Iwasaki (1937)	$\frac{\partial C}{\partial Z} = -\lambda_{O}C$	$\frac{c}{c_0} = c$
2	Mints (1951)	$\frac{\partial C}{\partial z} = \lambda C - \frac{a}{u} \sigma$	$\frac{c}{c_0} = \sum_{n=1}^{\infty} e^{-\lambda z} (\lambda z)^{n-1} \times $
			$T_{n} \in \mathbb{R}^{a \oplus a \oplus a}$ $T_{n} = T_{n-1} - (a \oplus a) = 2$ $T_{1} = e^{a \oplus a \oplus a}$
3	Shekhtman (1961)	$\frac{\partial c}{\partial z} = -\lambda_{c}(1 - \frac{1}{2})$ $j \sigma c$	$\frac{\lambda_{o} juc_{o}}{c_{o}} = \frac{\lambda_{o} z}{\lambda_{o} juc_{o}}$ $\frac{\lambda_{o} z}{e} + e$
4	Ives (1963)	$\frac{\partial c}{\partial z} = -(a - a)$ $b \sigma^{2})c$	$\frac{c}{c_0} = \frac{Be^{-az}}{(B^2 - 1 + e^{-2az})^{1/2}}$ $\frac{2uc_0e(ab)^{1/2}}{(ab)^{1/2}}$ $\frac{2uc_0e(ab)^{1/2}}{(ab)^{1/2}}$

A different approach was adopted by Mints (1951) and later by Litwiniszyn (1967). The rate expression is assumed to be

$$-\left(\frac{\partial C}{\partial z}\right)_{+} = \lambda C - \frac{\partial C}{\partial z} \qquad (2.9)$$

Here, a is the coefficient of filtration rate expression.

The first term of the equation represents particle deposition as before, whereas the second term is introduced to account for the scouring of deposits, evidence of which is given by the observation that in a shallow filter, the effluent was found to contain particle aggregates significantly greater than those present in the influent stream (Mints et.al., 1967). Mints also argued that improved filtration efficiency, due to the application of polyelectrolytes, can be attributed in part to the fact that polyelectrolytes increase the bonding strength among the deposits, therefore reducing the extent of scouring.

The shortcoming of these expressions is that all the model parameters can be determined only empirically. Some attempts have been made to develop generalized correlations for λ_0 . For example, Ives (1971) suggested the following form of correlation:

$$\lambda d_{g} = P_{1} \left(\frac{d_{p}}{d_{g}}\right)^{e_{1}} \left(\frac{k_{T}}{6\pi \mu a_{p}} u d_{g}^{e_{2}}\right)^{e_{2}} \left(\frac{2/\rho_{p} - \rho/a_{p}^{2} g e_{3}}{9\mu u}\right)^{e_{3}} \left(\frac{\rho u d_{g}^{e_{4}}}{\mu}\right)^{e_{4}}$$
(2.10)

Here, d_g is the grain diameter, P_1 is a coefficient, d_p is the suspended particle diameter, k is the Boltzmann's constant, P_1 is the absolute temperature, P_2 is the viscosity, P_1 eg, P_2 are exponents, P_3 is the

particle radius, $\rho_{\rm p}$ is the density of suspended particle, ρ is the density of liquid, and g is the acceleration due to gravity. However, there do not exist sufficient data or, more importantly accurate data to establish such a correlation. Rajagopalan and Tien (1977) also pointed out the lack of theoretical validity for an expression such as that of Eq. (2.10). Accordingly, the prediction of filter coefficients, as well as of the relevent functional expressions, must largely rely upon theoretical means.

2.1.2 Prediction of Pressure Drop

For a clean filter bed, the pressure drop versus flow rate relationship is governed by the Carman-Kozeny equation, that is

$$-\left(\frac{\partial p}{\partial z}\right) = \frac{150}{d_{q}^{2}} \mu u \frac{\left(1 - F\right)^{2}}{F^{3}}$$
 (2.11)

To account for the change in pressure gradient due to filter clogging, either one of the following expressions may be used:

or

$$\frac{(\partial p/\partial z)}{(\partial p/\partial z)}_{0} = 1 + F_{2}(\beta, \sigma)$$
 (2.12b)

Here, β is the parameter vector of function $F_1(\beta,\sigma)$ and $F_2(\beta,\sigma)$, and p is the pressure.

A number of specific functional forms have been proposed for F_1 or F_2 (Ives and Pienvichitr, 1965; Ives, 1969; Herzig et.al., 1970). Ives and Pienvichitr (1965) pointed out that most of these expressions can be derived from a general form:

$$F_{1}(\beta, \sigma) = \frac{1}{(1 - \beta_{2} \sigma)\beta_{1}} = 1 + \beta_{1} \beta_{2} \sigma + \frac{\beta_{1} + (\beta_{1} + 1)}{2} \beta_{2}^{2} \sigma^{2} + \dots$$
(2.13)

Here, β_1 and β_2 are components of β .

Although theoretical expressions similar to that of Eq. (2.13) have been obtained, these expressions are based on specific deposit morphology which may or may not be valid for the problem at hand. In practice the coefficients (β_1 and β_2 for example) have to be determined from experimental data.

If the specific functional form of F_1 is known, and furthermore if $\sigma(z,\Theta)$ is known from the solution of the conservation equation [that is, Eq. (2.4)] and the rate expression [Eq. (2.5)], the pressure distribution can be obtained from a simple integration as follows:

$$p - p_{o} = \left(\frac{dp}{dz}\right) \int_{0}^{z} F_{1}[\beta, \sigma(z', \theta)] dz' \qquad (2.14)$$

2.2 Theoretical Approach

The phenomenological equations discussed above describe the dynamic behavior of deep bed filtration in terms of model parameters and functions. The importance of estimating these quantities with sufficient accuracy is rather obvious. Since no generalized correlations for the estimation of these

quantities have been established, one has to resort to theoretical calculation. Furthermore, theoretical analysis has the added advantage of providing a more fundamental understanding of the deposition phenomenon.

The complicative of the filtration process has led some to believe that a complete theoretical formulation of filtration may not be attainable at all. Mintz (1966), reporting at the 1966 International Water Supply Congress, Barcelona, stated that:

"There are complicated interrelationships among many factors affecting the performance of rapid filters. These interrelationships may vary with seasonal changes in the quality of raw water, chemical treatment, output, and load changes. Therefore, it is apparent that an attempt to work out an exact mathematical description, with theoretical constants, of the filtration process to hold for any conditions of filter operation is bound to fail."

Despite of this generally accepted pessimistic view, it has been suggested by O'Melia (1965) that a reasonable understanding of the basic mechanisms involved in filtration process may be obtained by envisioning this process as involving two distinct steps: (1) the transport of the suspended particles to the immediate vicinity of the fil er grains, and (2) the attachment of particles to the filter grains or to the particles already deposited. This same approach has been successfully employed in the formulation of the coagulation process.

The transport step is a physical process and is controlled by physical filtration parameters such as flow rate, grain size and shape, bed porosity and depth, and the shape and density of the suspended particles. Particle attachment, however, is a colloid-chemical process and is affected by a variety of both chemical and physical parameters. Thus by considering both transport and attachment steps the effects of both physical and chemical variables can be incorporated in developing a combined physical-chemical filtration model.

2.2.1 The Transport Step

The principle involved in the theoretical calculations in quantifying the extent of transport of suspended particles in a filter bed is as follows. A filter bed can be viewed to be an assembly of particle collectors. Using the terminology of Payatakes et.al. (1973) a filter bed can be considered to be a series of Unit Bed Elements (UBE), each of which, in turn, is composed of a number of collectors. Since the thickness of a unit bed element AL is always small, Eq. (2.6a) can be applied to a UBE with the assumption that the filter coefficient remains constant throughout the element. Considering the ith UBE, let c_{i-1} and c_i be the concentration of the influent and effluent streams, respectively, the following result is obtained:

$$\ln \frac{c_{i-1}}{c_i} = \lambda \Lambda L \qquad (2.15)$$

Similarly, the capacity of a UBE to remove particulates from the fluid stream is characterized by its collection efficiency η^{\bullet} , defined by

$$\frac{c_{i-1} - c_{i}}{c_{i-1}} = \eta'$$
 (2.16)

Comparing Eqs. (2.15) and (2.16), we get

$$\lambda = \frac{1}{1} \ln \frac{1}{1 - \eta^{\frac{1}{2}}}$$
 (2.17)

Specification of geometrical configurations for the collectors present in a UBE is admittedly somewhat arbitrary. In principle, any model which adequately describes the flow field in porous media can be used. This possibility of multiple selection, however, is limited by practical considerations that only relatively simple geometrical entities should be used. The models employed by various investigators can be grouped into three categories: capillaric collector (Payatakes et.al., 1974a; Hung and Tien, 1976), spherical collector (Yao et.al., 1971; Spielmen and Fitzpatric, 1973; Payatakes et.al., 1974a,b; Rajagopalan and Tien, 1976, 1977), and the constricted tube collector (Payatakes et.al., 1974c, d).

Using the collector concept, the retention of particulate matter within a filter medium can be considered in terms of the deposition of particles from a suspension flowing past collectors of specified geometry. The mechanisms of deposition are known to be inertial impaction, sedimentation, interception, Brownian diffusion, and straining. For liquid systems, the effect of inertial impaction is negligible, and the relative importance of other mechanisms depends upon a number of variables, the most significant of which is perhaps particle size. Although explicit rate expressions of deposition for

some of the individual mechanisms are available, in most practical situations deposition takes place according to more than one mechanism.

The most versatile method for estimating the rate of particle deposition is the so-called trajectory calculation. As particles move toward a collector, their trajectories deviate from stream lines, and some of them may intersect with the collector. If one assumes that deposition occurs once a particle makes contact with the collector, the particle deposition flux can be estimated if particle trajectories are known. These trajectories can be determined in turn from the appropriate equations of particle motion, with the knowledge of the forces acting on the particle.

The idea of determining the rate of particle deposition from particle trajectories was first advanced 50 years ago in connection with air filtration (Sell, 1931; Albrecht, 1931). However, the possibility of extending this concept to liquid filtration was recognized only rather recently (O'Melia and Stumm, 1967).

A detailed discourse on the determination of particle trajectories is beyond the scope of the present thesis. To initiate trajectory calculation, the following procedures have to be followed:

- Specification of collector geometry, collector size and size distribution.
- Specification of flow field around or within the specified collector, and

3. Specification of forces acting on particles under consideration.

Thus, a variety of combinations of conditions can be used for the calculation of collection efficiency, a fact which accounts for the differences among the various studies on this subject carried out during the past decade. A summary of these studies is given in Table 2.2.

The particle trajectories are obtained from the integration of the appropriate equations of particle motion, which are obtained from the balance of forces and torques acting on the particle. The exact form of these equations varies with the geometry of the collector, but they are first order differential equations because of the omission of the inertial force.

Furthermore, the Brownian diffusion force cannot be included owing to its stochastic nature. The forces which have been considered are gravity, hydrodynamic drag (with or without wall correction), and different kinds of surface forces. The effect of interception is included as a boundary condition to determine particle deposition.

The pertinent equations of particle motion, irrespective of their specific forms, contain a large number of dimensionless parameters, a listing of which is given in Table 2.3. In general, these equations do not permit analytical solutions but can be solved effectively with a number of algorithms such as the fourth-order Runga-Kutta method or the Adams-Moulton method. However, for two cases, isolated sphere model (Rajagopalan and Tien, 1977) and the sphere-in-cell model (Rajagopalan and

Summary of results on trajectory calculations for deep bed filtration (Adopted from Tien and Payatakes, 1979) Table 2.2.

Model	Investigator	Remarks
Single-sphere model	Yao et.al. (1971)	Surface interaction not included; drag correction neglected
single-sphere model	Rajagopalan and Tien (1977)	Surface interaction with retardation effect for London force. Drag correction considered
Capillaric model	Payatakes et.al. (1974b)	Surface interaction with retardation effect fair London force. Drag correction considered
Capillaric model	Hung and Tien (1976)	Surface interaction and drag correction included; nonvanishing fluid velocity across collecting surface
Sphere-in-cell model (Happel's model)	Spielman and Fitzpatrick (1973)	Approximate fluid velocity expression valid for small particles. No retardation effect.
Sphere-in-cell model (Brinkman model)	Payatakes et. 1. (1974b)	Surface interaction and drag correction included
Sphere-in-cell model (Happel's model)	Rajagopalan and Tien (1976)	Surface interaction with retardation effect for London force and drag correction included
Constricted tube model	Payatakes et.al. (1974c,d)	Surface interaction with retardation effect for London force and drag correction included. Constricted nature of flow channels considered

Table 2.3. Dimensionless groups appearing in trajectory analysis*

Name	Symbol	Definition
Double layer group	$^{ m N}_{ m DL}$	κa
Electrokinetic group No. 1	N _E 1	$\kappa \bar{\epsilon} (\psi_{01}^2 + \psi_{02}^2)/12\pi \psi_{\infty}$
Electrokinetic group	N _{E2}	$2_{\psi_{01}} \psi_{02} / (\psi_{01}^2 + \psi_{02}^2)$
Gravitational group	$^{ m N}_{ m G}$	$2a_p^2(\rho_p - \rho)g/9\mu V_{\infty}$
London group	NLo	H/9πμ ap2 V∞
Relative size group	$^{ m N}_{ m R}$	a _p /a _c
Retardation group	^N Rtd	$2 \mu \pi a p / \lambda e$
Brownian diffusion group (Peclet number)	N _{Pe}	V_{∞} (2a _C)/D _{BM}

^{*} Here, κ is the double-layer reciprocal thickness, $\overline{\epsilon}$ is the dielectric constant, ψ_{O1} and ψ_{O2} are the surface potentials of particle and grain respectively, V_{∞} is the interstitial velocity of filter bed, H is the Hamaker's constant, a is the collector radius, λ_{e} is the wavelength of electron oscillation, and D_{BM} is the particle diffusion coefficient in liquid.

Tien, 1976), collection efficiency values obtained from numerical calculation have been correlated empirically with relevant dimensionless parameters, thus overcoming the major objection about the use of trajectory calculation for the estimation of collector efficiency. These expressions are

Sphere-in-cell model (Rajagopalan and Tien, 1976)

$$\eta_{o} = 0.72 A_{s} N_{Lo}^{1/8} N_{R}^{15/8} + 2.4 \times 10^{-3} A_{s} N_{G}^{1.2} N_{R}^{-0.4}$$
for $N_{R} < 0.09$ (2.18)

Here,

$$A_{S} = 2(1 - P)^{5}/W \tag{2.19}$$

$$P = (1 - F_0)^{1/3} = a_0/b$$
 (2.20)

$$W = 2 - 3P + 3P^5 - 2P^6$$
 (2.21)

Isolated sphere model (Rajagopalan and Tien, 1977)

$$\eta_{0} = N_{G} + 1.5 N_{R}^{2}$$
 (2.22)

The definitions of the dimensionless groups are given in Table 2.3. These expressions are based on results obtained under the assumption that the surface interactions (van der Wall's force and double layer force combined) are favourable.

The collection efficiency obtained from trajectory calculation is often referred to as the initial collection efficiency or clean collector efficiency. Significant particle deposition may change the collector configuration, alter its surface characteristics, and cause the flow field around the

collector to be different from that around a clean collector to such an extent as to render the collection efficiency calculated with the omission of these factors to be erroneous. The principle of trajectory calculation, however, remains valid. The problem is that of taking into account all these changes in the formulation of the trajectory equation.

At this stage it is important to note that Eq. (2.18) based on trajectory calculations, does not include several mechanisms which may be operative in deep bed filtration.

However, these mechanisms are incorporated in computing the transport efficiency of particle collection either empirically or based on theoretical calculations (Hall, 1957; Maroudas and Esienklam, 1965; Agrawal, 1966; Yao, 1968; Craft, 1969; Cookson, 1970; Fitzpatrick, 1972; Clint et.al., 1973; Wenk et.al., 1977).

2.2.2 The Attachment Step

The attachment step in filtration is studied using the similarity between coagulation and filtration. The resemblance between coagulation and filtration can be justified from the findings of Habibian (1971). Both process can be envisioned as involving a transport step and an attachment step.

The overall efficiency of coagulation can be determined from the rate at which particle collisions occur multiplied by a "collision efficiency factor" which represents that fraction of the total number of collisions which produce inter-particle attachment. It is plausible that the overall removal efficiency of a filter may be represented by the rate of transport of suspended particles to the filter grains multiplied by a

"holding efficiency" which represents the effective portion of contacts.

The attachment step is a colloidal-chemical process, and unfortunately the present knowledge of colloid chemistry does not provide a quantitative model of this step. Therefore, the similarity between the attachment step in filtration and coagulation cannot be shown in mathematical terms. The concept, however, becomes more evident by considering that in both processes the particle should be made "sticky" so that they may attach to each other or to the filter grains upon contact. This means that the potential energy barrier between the particles or between the particles and filter grains should be reduced or nullified.

At the beginning of a filtration cycle the energy barrier between the particles and filter grains can control the attachment of particles to filter grains. However, as filtration proceeds, the suspended particles coat the filter grains and further removal occurs primarily by the attachment of particles in suspension to particles already deposited on filter grains. Therefore, shortly after the commencement of a filtration cycle, the magnitude of the energy barrier between particles in suspension and particles deposited on filter grains controls the particle attachment in the filtration process. This same potential also governs interparticle attachment in the coagulation process. The role of attachment step in filtration has been qualitatively studied (Habibian and O'Melia, 1975).

However, the quantification of this step remains out of reach with the present state of knowledge.

2.2.3 Dynamics of Deep Bed Filtration Based on Theoretical Approach

The retention of particulate and colloidal matters within a filter bed causes changes in the microstructure of the filter medium. As a result, the behavior of the flow of fluid through the medium and the deposition of particles from suspensions to filter grains can be significantly affected.

Qualitatively speaking, the major changes resulting from particle deposition involves the effective size and geometry of filter grains, the surface characteristics of the grains, the porosity, and the effective porosity of the bed. The last quantity is defined as the fraction of the connected void space which is open to suspension flow. This is an important variable in the understanding of the effect of deposition on filter performance, since particle deposition may result in the blocking of certain flow passages of the bed. A complete filtration theory should provide information on these changes as functions of operating and system variables. Once these changes are known, it would be possible at least in principle, to account for these changes in predicting filtration rates and pressure drop requirements.

The development of modern filtration theories, of course, has not reached such a stage as to permit a complete and quantitative description of the effect of particle deposition.

A number of investigators (Camp, 1964; Mohanka, 1969; Deb, 1969; Ives, 1969; Sakthivadivel et.al., 1972) have presented relationships between the local pressure gradient of a clogged filter bed and the extent of particle deposition. The starting point was usually the Carman-Kozeny equation. The effect of deposition was assumed to increase the grain size and to decrease the local porosity on the basis that deposition over filter grains is uniform, resulting in the formation of a smooth deposit layer outside the grains. In general, their results can be expressed as

$$\frac{\partial p/\partial z}{(\partial p/\partial z)} = \prod_{i=1}^{M} (1 - p_i \sigma)^{a_i}$$
 (2.23)

The number of terms involved M, the coefficients p_i^* , and the exponents a_i 's depend upon the particular model used to characterize the filter bed. Similarly, the removal efficiency of filters as the filtration progresses is related to the specific deposits and the porosity of the deposits.

The selection and application of these expressions for predicting filter performance cannot be made without additional evidence or assumption on deposit morphology. A complete solution to the problem requires a theory which provides detailed information about the deposition process, including the formation and growth of particle deposits as a function of time. Such a theory is not yet available, although some progress has been made along this direction. Payatakes and Tien (1964) and Payatakes (1977) have presented mathematical models for aerosol

particle deposition with dendrite like pattern and related collection efficiency, and pressure drop as functions of the degree of deposition. It is likely that the same approach can be applied to hydrosol systems. Tien et.al.(1977) and Wang et.al. (1977) argued that deposition phenomena, in general, can be studied in terms of the two properties which are characteristics of deposited particles and approaching particles, respectively. The shadow effect refers to the fact that once a particle is captured by a collector, certain parts of the collector surface near the deposited particle would no longer be accessible to approaching particles (and those areas are called shadow areas). The degree of uniformity of deposited matter (or the lack of it) is a direct consequence of the magnitude of these shadow areas. The morphology of particle deposits can be determined by the fact that the spatial distribution of particles in a dilute suspension follows Poisson's law and the presence of deposited particles allows approaching particles to be collected by the collector as well as by the already deposited particles.

This principle was adopted by Beizaie (1977) in his study of deposition on single isolated spherical collectors. His results indicate that the deposition process, in general, consists of three steps. The first, or the initial stage, may be called the clean collector stage during which the presence of deposited particles have negligible effect. The second stage, or the dendrite growth stage, is characterized by the formation and growth of particle dendrites. During this stage, an

increasing amount of particle deposition is affected by deposition on deposited particles. The third stage of the process is termed the open structured solid growth stage. Particle collection is entirely due to deposition on deposited particles, and individual particle dendrites become less distinguishable as they become merged and interconnected. A direct application of Beizaie's results to filter clogging, of course, would be inappropriate, since the use of the isolated sphere model precludes consideration of the effect due to the presence of neighbouring grains. However, with the use of a more realistic porous media model Beizaie's method on deposition dynamics can be applied advantageously to the study of filter clogging.

With the same concept of dendrite formation, Ali (1977) proposed a formulation for the change in single collector removal efficiency as follows

$$\eta_{r} = \eta \alpha + N \eta_{p} \alpha_{p} \left(\frac{d_{p}}{d_{e}}\right)^{2} \qquad (2.24)$$

Here, η_{r} is the single collector removal efficiency at any time after the start of filtration process, N is the number of retained particles acting as collectors, η is the collision efficiency of the clean media grain, α is the ratio of particles adhering to particles colloiding with the filter grain, d_{c} is the diameter of the media grain, and η_{p} α_{p} are the corresponding η , α values for particle to particle collision and attachment respectively.

Further, for estimating the value of N at any time, Ali (1977) proposed the following equation:

$$\frac{\partial N}{\partial t} = \beta!! \, \eta \, \alpha \, \nabla n \, \frac{\pi}{4} \, (c_c)^2 \qquad (2.25)$$

Here, β "is the fraction of the particles removed which will act as collectors, n is the local concentration of particles in suspension, and \boldsymbol{v}_0 is the superficial velocity.

Since, n is a function of both filter depth and time, N will also be a function of both filter depth and time. The above expression fails to consider the variation of N along the filter depth. Further, Eq. (2.25) indicates that N would keep on accumulating infinitely and so also the $\eta_{\rm r}$, and hence the overall efficiency of the filter bed, which is very unlikely. This descripancy is because of neglecting the effect of shadow areas in formulating the aforementioned model.

2.3 Summary

Recent advances in the study of deep bed filtration have shown that inspite of the inherent complexities of the process, the problem can be studied fruitfully based on fundamental considerations. Resurgent research efforts of the past two decades have already yielded important results of practical significance. The review presented, examines both the phenomenological and theoretical studies conducted during recent years. It reveals that deep bed filtration is a challenging and fascinating subject of study and warrents further attention and effort from scientists and engineers.

The main problems which are relevant to a fundamental understanding of deep bed filtration are the nature and the conditions leading to the retention of particles throughout a filter bed, the change of the filter media structure due to

deposition, and its effect on filter performance. A reasonably complete understanding of the pertinent phenomena is essential for the establishment of a comprehensive deep bed filtration theory which can be used as a basis of rational design.

It appears that the deposition phenomena, in general, can be studied in terms of the two properties which are characteristic of deposited particles and approaching particles. The morphology of particle deposits can be determined by the fact that the presence of deposited particles allows approaching particles to be collected by the collector as well as already deposited particles. Thus the formulation based upon this concept should be able to predict the filter performance in accordance with the observation made on deep bed filtration. It is important to note that such a formulation must incorporate the effect of shadow areas.

3. SCOPE OF THE INVESTIGATION

Recent advances in the study of deep bed filtration have shown that in spite of the inherent complexities of the process, the problem can be studied fruitfully based on fundamental consideration. Many attempts have been made towards the simulation of the dynamic behavior of deep bed filter. The major limitation of the existing simulation procedures is the requirement of extensive pilot plant studies for the determination of the certain coefficients such as filter coefficient, specific deposits, porosity of the filter bed, self porosity of the deposited material etc. Further, the formulations used in such simulation techniques neglect the physical and chemical characteristics of the particles forming the deposited material in the filter. Though the importance of physical and chemical properties of the deposited matter was realized long back, these could not be incorporated in the formulations because of the inherent limitation of estimating such properties. particular, the lack of data on particle size distribution has hindered the theoretical studies of filtration process and prevented the use of suspended particle size as a basic parameter in design. However, the advent of particle counters and their successful use in the control of water treatment process is expected to overcome this major difficulty (Tate and Trussell, 1976; Wright, 1979). Consequently the present investigation is undertaken with the basic motive of developing a conceptual formulation for predicting the filter performance.

The work is concerned with the development of simulation procedure capable of predicting the dynamic behaviour of a deep bed filter over the broadest practicable range of the pertinent variables involved, including, in particular, the suspended particle size The method presented here is developed by assimilating available quantitative results relating to porous media flows, and to filtration, in the context of conceptual framework. The main hypothesis can be stated as follows:

"The removal of suspended particles in filtration is a two step process. The first step accounts for the transport of suspended particles to the filter media grain or already deposited particles. The second step incorporates the attachment of such particles to media grain or previously deposited particles. This assumes that the deposited particles or the retained particles may also act as collectors."

This picture of the process is supportable on the basis of observed filter behaviour and does, moreover, provide the means for integrating results into the overall simulation scheme. In general the objective of this research is to formulate and verify the new conceptual model with aforementioned hypothesis. Specifically, the present study is directed to the following aspects of the overall problem.

- 1. To study the role of suspended particles retained in a filter bed with respect to removal efficiency and head loss development, and to investigate the influence of the size of these particles on filter performance.
- 2. To propose a mathematical model for removal efficiency following practice in aerosol and water filtration using collector theory.

- 3. To modify the Carman-Kozen y head loss equation for clean filters to predict the head loss development as the filtration progresses.
- 4. To verify the proposed formulation for removal efficiency and head loss developed using existing data and the data obtained in the present investigation, and thereby evaluating various physical and chemical parameters deciding water and wastewater filtration as an unit operation.
- 5. To simulate the filter performance for various physical and chemical parameters based on proposed mathematical model.
- 6. To propose a mathematical equation for the depth of clogging front which would give the depth of floc penetration relating to head loss developed as the filtration progresses.
- 7. To study the temporal variation of the depth of clogging front for various physical and chemical parameters influencing filtration process.

4. MODEL FORMULATION

Filtration is a complex process due to the diversity of the mechanisms involved. A reliable mathematical description of the removal of suspended particles within a filter bed is necessary to obtain a reasonable understanding of the mechanisms involved. The prerequisite to such an approach is the knowledge of the mode of deposition of suspended particles within a filter.

The mode of deposition of suspended particles within a filter bed is believed to be in the form of chainlike particle dendrites. Tien et.al. (1977) have presented a theory for the formation and growth of such particle dendrites on a collector placed in an aerosol or hydrosol system. They attribute such a formation to the finiteness of the particle size which creates shadowing effect. Due to the formation of a shadow area particles find it difficult to deposit in this shadow area and hence tend to attach to the previously retained particles rather than the filter grain. Yao et.al. (1971) have also mentioned the possibility of such particle attachment in water filtration. However, the possibility of the existence of long particle dendrites in water filtration is a subject of controversy among the researchers involved in modelling the deep bed filtration. Nevertheless, the fact that the filtration efficiency changes as the filtration progresses clearly indicates that the deposited particles play a significant role.

Most of the existing mathematical models for predicting the dynamics of deep bed filtration attribute changes in filter

performance to the changes in bed porosity and the self porosity of the deposits. These models neglect the physical and chemical characteristics of the particles forming the deposits in the filter. The only term which may represent the characteristics of the particles is the self porosity of deposits. For equal amounts of removal, however, it is intuitive that self porosity of the deposit is independent of particle In other words, the head loss resulting from equal removal size. of two suspensions of different particle size will be the same, whereas the experimental data of Habibian (1971) show the reverse. The filtration of suspension having particle size of 0.1 µm resulted in much higher head loss than those having 1 and 7.6 µm particle size. Further, if decreased porosity and pore size are the main important factors responsible for the changes in filtration efficiency, then filtrate quality should continuously improve, provided there is no reentrainment of the deposited particles. However, many experiments conducted under different set of conditions by Habibian (1971) show the deterioration in effluent quality right from the beginning of the filtration run when the reentrainment of the deposited particles is not expected. This discrepancy between experimental observations and predicted filter performance using existing models is due to the inability of these models to incorporate the physical and chemical characteristics of the particles forming the suspension into the equations for particle removal and head loss.

In the present research a new conceptual model has been formulated for predicting the filter effluent quality and head

loss development as the filtration progresses relating to various physical and chemical parameters. The model is formulated with the concept of deposited particles acting as collectors taking into consideration the effect of shadow areas. The model formulation is described in the subsequent sections.

4.1 Terms Used

For the purpose of clarity, some of the terms are described prior to the model formulation.

Single Collector Efficiency: In the filtration literature, the term single collector efficiency is used interchangeably to represent the single collector removal efficiency without distinction. Most of the previous work relating to the use of this term deals with the transport aspect of the filtration process. Therefore, to be consistent, the term single collector efficiency represents the single collector collision efficiency. Single Collector Removal Efficiency: The term single collector removal efficiency is used to represent the actual removal by the collector accounting for both the transport and its attachment steps.

Single Collector: A single collector herein is referred to the assembly consisting of a filter grain and that number of particles attached to it which act as collectors. At the start of the filtration process (i.e., at time equal to zero when no particles have been attached to the filter grains) the assembly consists of only the filter grains themselves. The term single collector used herein is, therefore, inconsistent with the use

of the term by other investigators who use the single collector to represent a filter grain in studying the clean filter performance.

4.2 Assumptions and Their Justification

To study the role of retained particles in a filter, a mathematical model for the filtration of dilute suspensions through a filter bed is developed for a monosized filter media and particles, both spherical in shape. To facilitate mathematical manipulation, following assumptions are made.

- The flow around the collector remains unaltered as the particles are removed.
- 2. The diameter of the single collector is equal to the diameter of the filter grain and that the diameter of the retained particle acting as collector is equal to its own size. The assumptions are justified as long as the filter media is much greater in diameter than the diameter of the suspended particles (Yao, 1968).
- 3. The porosity of the filter bed is considered to remain fairly constant as the filtration proceeds. This assumption is generally made by other investigators in water filtration in dealing with the removal efficiency of the process. Herzig et.al. (1970), discussing the assumption, have stated that it may result in an error of the order of 0.3 percent in dilute suspensions.

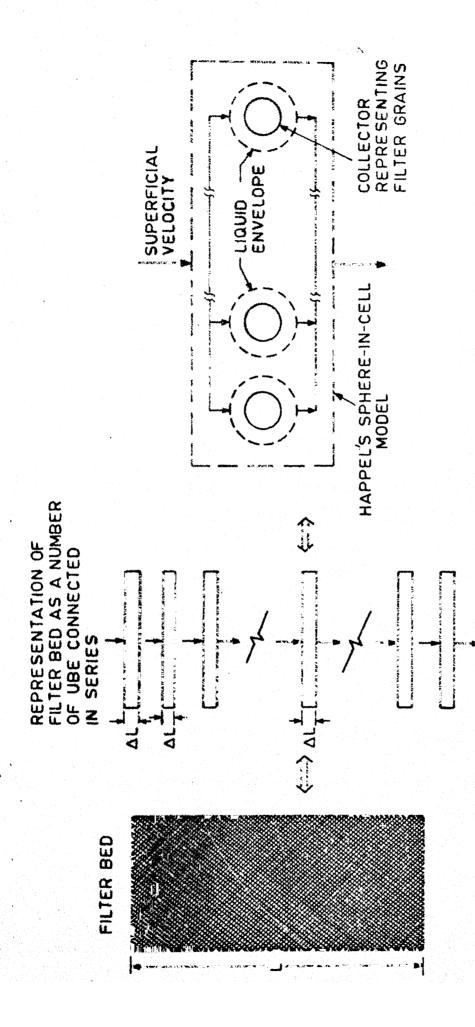
 Payatakes et.al. (1974b), who used capillaric and Brinkman's model to calculate the head loss increase during the course of filtration, have reported that the

calculated head loss values were less by two to three orders of magnitude then the observed ones even taking into account the decrease in the bed porosity. This indicates that in dealing with dilute suspensions, the assumption of constant porosity is not critical, at least for some time after the start of filtration.

- 4. The flow through the filter is laminar. Justifying this assumption in water filtration, Yao (1968) states that for filtration velocities from 0.136 to 0.272 cm/sec and media sizes upto 1.0 mm, the Reynolds number based on media size varies approximately from 0.5 to 5, whereas the transition from laminar to turbulent may begin at Reynolds number from 10 to 113.
- 4.3 Model Representation of Filter Bed

To provide a physically realistic model as the basis for quantitative descriptions of the various processes of interest which occur in the porous medium, the concept of Unit Bed Element (UBE) and the unit collector proposed by Payatakes et.

al. (1973) is used. Thus, the filter bed is postulated to consist of a number of unit bed elements, with a physical height of AL, connected in series. Each UBE in turn is assumed to consist of a number of particle collectors. The capacity of the unit bed to remove particulate matter can thus be defined as the fraction of suspended particles entering the UBE removed. The general idea of depicting a filter bed as a series of UBE's is illustrated in Fig. 4.1.



Representation of filter bed as an assembly of collectors. Fig. 4.1.

Specification of geometrical configurations for the collectors present in a UBE is admittedly somewhat arbitrary. In principle, any model which adequately describes the flow field in the porous media can be used. This possibility of multiple selection, however, is limited by practical considerations that only relatively simple geometrical entities should be used. The models employed by various investigators are reported in Section 2.2.1. Because use of the spherical collector leads to significant simplifications, it remains as an attractive collector configuration, affording considerable computational convenience as well as leading to physically meaningful results when used in appropriate context. Further Rajagopalan and Tien (1976) reported that the calculated collection efficiency values based on different collector configurations turn out to be comparable in magnitude. As a consequence of the foregoing considerations, it is proposed to use the Happel's porous media model to compute the collision efficiency in this study.

4.4 Hypothesis of Deposition Process

The importance of the knowledge of deposit morphology in understanding the effect of particle deposition is rather obvious. Therefore any theory presented for the performance of the process must account for the manner in which the particles are deposited within a filter.

In the present work, the deposition phenomenon is studied in terms of the two properties which are characteristics of

deposited particles and approaching particles respectively. It is postulated that some of the retained particles within a filter can act as collectors along with the filter grains. Further, once a particle is captured by a collector, certain parts of the collector surface would no longer be accessible to approaching particles. In other words the deposition process may be viewed as follows.

"Initially when the filter bed is clean, the deposition process is controlled by the interaction between the suspension particles and the media grain. As the filtration progresses, deposited particles cover certain parts of the media grain and the deposition is controlled by the interaction between media grain and suspension particles, and deposited particles and suspension particles for the uncovered and covered portion of the media grain respectively. For the particles which are in direct contact with the media grain, the transport step would be controlled by the size of the grain and suspension particle while the attachment step would be controlled by the characteristics of deposited particle and approaching particle for the interaction between deposited particles and suspension particles. However, the portion of the retained particles which are acting as collectors and are deposited on the retained particles, both transport and attachment would be controlled by the properties of deposited particles and suspension particles."

4.5 Development of the Model

4.5.1 Prediction of Removal Efficiency

Following the practice in aerosol and water filtration (Friedlander, 1958; Yao et.al., 1971), the single collector efficiency $\eta_{_{\rm C}}$ can be obtained as follows

 η_{c} = Rate at which particles strike the collector

Considering a spherical collector of size 'd $_{\rm C}$ ', the projected area normal to the flow is

$$= \frac{\pi}{4} d_C^2$$

The rate at which particles move toward the collector is, therefore

$$= v_o n \frac{\pi}{4} d_c^2$$

Since the collector consists of a filter grain and that number of particles attached to it which act as collectors (N), the single collector efficiency can be rewritten as follows.

Rate at which rate at which particles particles strike + N X strike a retained particle the filter grain acting as collector $\eta_{\rm C} = \frac{\text{the filter grain}}{\text{V_on } \frac{\pi}{4} \, \text{d}_{\rm C}^2}$

Rate at which particles strike particles strike a retained part the filter grain
$$v_0$$
 n $\frac{\pi}{4}$ d v_0 Rate at which particles strike a retained part v_0 n $v_$

or

$$\eta_{c} = \eta + N \eta_{p} \left(\frac{d_{p}}{d_{c}}\right)^{2} \tag{4.1}$$

Accounting for the attachment step, the single collector removal efficiency ' $\eta_{\rm r}$ ' can be expressed as

$$\eta_{r} = \eta \alpha \left(d_{c}^{2} - \beta_{c} N d_{p}^{2} \right) / d_{c}^{2} + \beta_{c} N \eta \alpha_{p} \left(\frac{d_{p}}{d_{c}} \right)^{2}$$

$$+ (1 - \beta_{c}) N \eta_{p} \alpha_{p} \left(\frac{d_{p}}{d_{c}} \right)^{2} \qquad (4.2)$$

Here, β_C is the fraction of retained particles acting as collectors which would contribute for the surface coverage of media grains, and α and α_p are defined following the practice in coagulation as follows.

Number of collisions between filter grain and suspended particles which result in attachment Number of collisions which occur between filter grain and particle

and

Number of collisions between retained particles acting as collectors and suspended particles which succeed in attachment

Number of collisions which occur between retained particles acting as collectors and suspended particles

In other words, α and α_p can be called particle to filter grain and particle to particle attachment coefficients respectively.

In Eq. (4.2) the factor $[(d_c^2 - \beta_c \ N \ d_p^2)/d_c^2]$ is introduced for the reduction in surface coverage of the media grain which would not be available for contact of suspended particles. The second term in Eq. (4.2) represents the removal efficiency because of the retained particles acting as collectors which contribute for the surface coverage of the media grain. For such retained particles the collision efficiency is η and the contact efficiency is α_p . The third term represents the removal efficiency of the retained particles acting as collectors which would not contribute for the surface coverage of the media grain or which are not in direct contact with the media grain. The collision and contact efficiencies for these particles will be η_p and α_p respectively.

The single collector efficiency of a filter grain is expressed as

 η = Rate at which the particles strike the filter grain v_o n $\frac{\pi}{4}\,d_c^2$

or rate at which the particle strike the filter grain is

$$\eta \ \mathbf{v}_{0} \ n \ \frac{\pi}{4} \ \mathbf{d}_{C}^{2}$$

If α is the particle to filter grain attachment coefficient, the rate of removal of particles by a single filter grain is

$$\eta \alpha \quad \mathbf{v}_{\mathbf{p}} \quad \mathbf{n} \quad \frac{\pi}{4} \quad \mathbf{d}_{\mathbf{p}}^{2}$$

Similarly, the rate of removal of particles by retained particles acting as collector is

$$\eta_p \alpha_p v_o n \frac{\pi}{4} d_p^2$$

The change in number of collector particles on a single filter grain can be written as follows.

Change in number of collector particles on a single filter grain

- = Rate of removal of particles by single filter grain
 - + N X rate of removal of particles by retained particles on filter grain acting as collectors
 - N X rate of particles removed which would contribute for the reduction in effective area of the filter grain
 - N² X rate of particles removed which would contribute for the reduction in effective area of the retained particles acting as collectors

=
$$[c_1 + N(c_3 - \beta_c c_3) - N^2 c_4]$$
 n

 $-N^2 C_2 \beta_D] n$

Here, β_p is the fraction of removed particles which would contribute for the reduction in effective area of the retained particles acting as collectors.

$$C_{1} = \eta \alpha V_{0} \pi \frac{d_{C}^{2}}{4}; C_{2} = \eta_{p} \alpha_{p} V_{0} \frac{\pi}{4} d_{p}^{2};$$

$$C_{3} = \frac{\eta}{\eta_{p}} C_{2} \beta_{c} + (1 - \beta_{c}) C_{2}; C_{4} = C_{2} \beta_{p}.$$

Considering an extremely thin UBE of thickness ' ΔL ' of the filter bed, and making the mass balance for N, the following expression can be obtained.

$$\frac{\partial N}{\partial t} + V_0 \frac{\partial N}{\partial L} = \left[C_1 + N(C_3 - \beta_C C_3) - N^2 C_4\right] n \qquad (4.3)$$

The removal efficiency of the filter bed can be determined by considering an UBE of thickness 'AL' of the filter bed. The number of single collectors in this layer

$$= \frac{A(1 - F) \Delta L}{d^{3}}$$

$$\pi \frac{c}{6}$$

Here, A is the area of the filter bed.

The removal by a single collector of removal efficiency $\eta_{\mbox{\scriptsize r}}$ from definition

$$= \eta_r v_o n \frac{\pi}{4} d_c^2$$

Therefore the removal by the UBE of thickness 'AL'

$$= \frac{3}{2} \eta_{r} A V_{o} n \frac{(1 - F)}{d_{c}} \Delta L$$

Making the mass balance for the suspension as it flows through the UBE under consideration, a mass balance equation can be written as

Rate of accumulation = Rate of input - Rate of output - Removal

If 'n' is the number of particles in suspension entering the UBE, the changes in number as they flow through the UBE is

$$n + \frac{\partial \mathbf{L}}{\partial \mathbf{n}} \wedge \mathbf{L}$$

and

Rate of input =
$$A V_0$$
n

Rate of output =
$$A V_0(n + \frac{\partial n}{\partial L} \Delta L)$$

Rate of accumulation =
$$A \triangle L \frac{\partial n}{\partial t}$$

In mathematical terms the mass balance equation becomes

$$A \Delta L \frac{\partial n}{\partial t} = A V_{o} n - A V_{o} (n + \frac{\partial n}{\partial L} \Delta L) - \frac{3}{2} \eta_{r} A V_{o} n \frac{(1-F)}{d_{c}} \Delta L$$

or

$$\frac{\partial n}{\partial t} = - V_0 \frac{\partial n}{\partial L} - \frac{3}{2} \eta_r V_0 n \frac{(1-F)}{d_C}$$

or

$$\frac{\partial n}{\partial t} + V_0 \frac{\partial n}{\partial L} \sim \frac{3}{2} \frac{(1-F)}{d_c} V_0 n \eta_r = 0$$
 (4.4)

Eqs. (4.2), (4.3) and (4.4) comprise a mathematical model to describe the removal efficiency of a filter bed in time and space. Their solution results in the removal efficiency of a filter bed. The exact solution of the above equations is not possible. Simplifying techniques are used to obtain a reasonably accurate solution. In this η_r and n are considered as step functions rather than continuous functions of time and depth. A new algorithm has been developed to solve these equations employing numerical methods. The details of the solution technique are presented in Appendix A.

4.5.2 Prediction of Head Loss Development

The development of head loss (h_f) is based on the well established Carman-Kozeny equation for head loss in a clean filter (h_{fo}) and can be written as

$$\frac{h_{fo}}{L} = K' \frac{\mu}{\rho} \frac{V_o}{g} - \frac{(1 - F_o)^2}{F_o^3} (\frac{A_c}{V_c})^2$$
(4.5)

Here, $A_{\rm C}$ and $V_{\rm C}$ are the surface area and volume of filter grains, and $K^{\rm I}$ is an empirical constant.

As the filtration proceeds, the suspension particles are deposited in the filter bed and thereby increases the surface area and volume within the filter. If the retained particles in time t contribute additional surface area \mathbf{A}_p and volume \mathbf{v}_p to the filter, the Carman-Kozeny equation becomes

$$\frac{h_f}{L} = K^{1} \frac{\mu}{\rho} \frac{V_o}{g} \frac{(1 - F)^2}{F^3} (\frac{A_c}{V_c} + \frac{A_p}{V_p})^2$$

or

$$\frac{h_f}{L} = K' \frac{\mu}{\rho} \frac{V_o}{g} (1 - F)^2 \left[\frac{\pi d^2 N_c + \beta' \pi d^2 N_p}{\frac{\pi}{6} d^3 N_c + \frac{\pi}{6} d^3 N_p} \right]^2$$
(4.6)

Here, N_c and N_p are the number of filter grains and retained particles in the unit volume of the bed respectively, h_f is the head loss after time t, and β' is that portion of the particles which contribute to the additional surface area.

The Eq. (4.6) can be rewritten as

$$\frac{h_{f}}{L} = 36 \frac{K'}{\rho} \cdot \frac{\mu}{g} \cdot V_{o} \frac{(1 - F)^{2}}{F^{3} d_{C}^{2}} \left[\frac{1 + \beta' \frac{N}{N} (\frac{d}{d})^{2}}{1 + \frac{p}{N_{C}} (\frac{d}{d})^{2}} \right]^{2}$$

$$(4.7)$$

Due to non-uniform deposition of particles in different layers of the bed, $\frac{h_f}{L}$ in each layer will be different. The filter depth may be divided into a reasonable number of layers and $\frac{h_f}{L}$ can be calculated in each layer. The sum of $\frac{h_f}{L}$ for all layers will result in the total head loss across the filter bed. N_p in each layer can be calculated from the removal efficiency.

4.6 Modification of the Model to Incorporate Varying Porosity

The model developed in the previous section, is based on the assumption that the porosity remains constant throughout the filtration process. Though this assumption is justified in case of dilute suspensions, to be more realistic the variation in porosity should be considered in the model formulation. The variation in porosity is incorporated by assuming that Eqs. (4.2), (4.3), (4.4), and (4.7) are valid only for a very small time interval At in which the porosity remains constant. After every time interval the porosity value is modified by AF, as follows:

$$F_{j+1} = F_0 - \Delta F_j \tag{4.8}$$

Here, F_{j+1} is the porosity in the $(j+1)^{th}$ time interval and $^{\Delta F}_{j}$ is the change in porosity in the $(j+1)^{th}$ time interval compared to initial porosity.

The change in porosity is computed by the volume of the deposited particles per unit volume of the filter bed as expressed by the following equation

$$\Delta \mathbf{F_j} = \sum_{\mathbf{i}}^{\mathbf{j}} (\mathbf{n_{i_j}} - \mathbf{n_{e_j}}) \frac{\pi}{6} d_{\mathbf{p}}^3$$
 (4.9)

Here, $n_{\mathbf{j}}$ and $n_{\mathbf{e}\mathbf{j}}$ are the influent and effluent particle concentrations respectively.

The porosity for the (j+1)th time interval can be written as

$$F_{j+1} = F_0 - \sum_{i=1}^{j} (n_{i,j} - n_{e,j}) \frac{\pi}{6} d_p^3$$
 (4.10)

Thus taking the appropriate value of porosity, the assumption of constant porosity can be eliminated in computing removal efficiency and head loss d velopment by Eqs. (4.2) to (4.4), and Eq. (4.7) respectively.

4.7 Modification of the Model for Varying Particle Sizes in the Suspension

The model developed in Section 4.5 is valid only for monosized particles in the suspension. However, the suspended particles present in either water or wastewater are of varying sizes. In order to apply the model developed to the realistic situations certain modifications are essential. The model for

monosized particles in suspension may be extended to varying particle sizes as follows.

Consider that the influent suspension contains m particle sizes having diameters d_{p_1} , d_{p_2} , ..., d_{p_n} in concentrations d_{p_1} , d_{p_2} , ..., d_{p_n} in concentrations

$$n_{o_1} + n_{o_2} + \cdots + n_{o_m} = n_{o_m}$$

or

$$\sum_{j=1}^{m} n_{0j} = n_{0} \tag{4.11}$$

For the jth particle size Eq. (4.2) may be written as

$$\frac{1}{2} \int_{\mathbf{r}}^{\mathbf{r}} d\mathbf{r} d\mathbf{$$

Here, subscripts i, j refer to the i th and j th particle sizes respectively.

The equation for computing the number of retained particles acting as collectors of the jth particle size may be obtained from Eq. (4.3) as follows.

$$\frac{\partial N_{j}}{\partial t} + V_{0} \frac{\partial N_{j}}{\partial L} = C_{1} \frac{n_{j}}{n_{j}} + \sum_{i=1}^{m} N_{i} (C_{3} - \beta_{c} C_{3}) n_{j} \\
- \sum_{i=1}^{m} N_{i}^{2} \cdot C_{4} n_{j} \frac{n_{j}}{j=1}$$
(4.13)

Here,

$$c_{1_{j}} = \eta_{j} \alpha_{j} v_{o} \pi \frac{d^{2}}{4};$$
 $c_{2_{i,j}} = \eta_{p_{i,j}} \alpha_{p_{i,j}} v_{o} \frac{\pi}{4} d^{2}_{p};$

$$C_{3_{i,j}} = \eta_{p_{i,j}}^{n_{j}} C_{2_{i,j}} \beta_{c} + (1 - \beta_{c}) C_{2_{i,j}} ; C_{4_{i,j}} = C_{2_{i,j}} \beta_{p}$$

$$\frac{\partial n_{j}}{\partial t} + V_{0} \frac{\partial n_{j}}{\partial L} + \frac{3}{2} \frac{(1 - F)}{d_{c}} V_{0} n_{j} \eta_{r_{j}} = 0$$
(4.14)

Eqs. (4.12), (4.13), and (4.14) comprise a mathematical model to describe the removal efficiency of a filter bed in time and space for the j th particle. The overall effluent quality may be expressed as

$$n = n_1 + n_2 + \dots + n_m$$

or

$$n = \sum_{j=1}^{m} n_j \tag{4.15}$$

The head loss development may be predicted by the following equation which can be obtained from Eq. (4.7).

$$\frac{h_{f}}{L} = 36 \frac{K'}{\rho} \cdot \frac{\mu}{g} \cdot V_{o} \frac{(1-F)^{2}}{F^{3}} \frac{1+\beta'}{c^{2}} \sum_{\substack{N=1 \ N \ 2}}^{m} \frac{v_{pj}}{N} \frac{d_{pj}}{d_{c}} \frac{2}{(d_{c})^{2}}$$

$$1 + \sum_{j=1}^{m} \frac{v_{pj}}{N} \frac{d_{pj}}{d_{c}} \frac{3}{(d_{c})^{2}}$$

$$1 + \sum_{j=1}^{m} \frac{v_{pj}}{N} \frac{d_{pj}}{d_{c}} \frac{3}{(d_{c})^{2}}$$

$$(4.16)$$

The verification of the proposed model for removal efficiency and head loss development using the data available in the literature and the experimental investigation conducted in this research is described in Chapter 6.

5. EXPERIMENTAL METHODOLOGY

5.1 Scope

The validity of the model and the proposal based upon it were evaluated by conducting appropriate experiments to supplement the data available in literature. These experiments are discussed in detail in Chapter Six of this thesis.

The effect of different particle sizes in the suspension on filter performance was investigated by conducting laboratory scale filtration experiments in both regions of filtration and in the critical suspended particle size range. Alum was used for precoating the media and destabilizing the suspended particles. Coagulation experiments were conducted to estimate the appropriate dose of alum for destabilizing the suspended particles in filtration experiments.

To facilitate the discussion of the apparatus, materials, and procedures, these experiments are divided into two groups: (1) the filtration experiments which were designed to investigate the influence of suspended particle sizes and their distribution on removal efficiency and head loss development, and (2) the destabilization experiments, which were conducted to estimate the appropriate alum dose to be used in filtration experiments. In subsequent sections of this chapter the apparatus, materials, and procedures used in these investigations are described.

5.2 Filtration Experiments

Many factors affect water and wastewater filtration and require control in filtration research. These factors can be categorized as follows:

- A. Characteristics of the filter bed
 - (a) **s**ize and shape of the media grains
 - (b) bed depth
 - (c) bed porosity and pore structure
 - (d) surface characteristics of the filter media
- B. Characteristics of the suspension to be treated
 - (a) size and shape of the suspended particles
 - (b) density of the suspended particles
 - (c) surface characteristics of the suspended particles
 - (d) concentration of the suspended particles
 - (e) chemical characteristics of the water or wastewater(e.g., pH, ionic strength etc.)
 - (f) chemical characteristics of the coagulant or
 "filter-aid" (e.g., charge, molecular weight etc.)
- C. Characteristics of the operation of the filter
 - (a) filtration rate
 - (b) direction of flow
 - (c) backwashing procedures.

In this research, characteristics of filter bed and its operation were kept constant in most of the experiments.

Emphasis was placed on the characteristics of the particles to be filtered. More specifically, the filtration of suspended

particles in both regions of filtration as well as in the critical range was studied when present separately and in different combinations.

5.2.1 Characteristics of the Filter Beds and Their Operation:

The filter apparatus (Fig. 5.1) employed in this investigation was principally designed to provide for testing the proposed model. In few experiments it was decided to employ two filter beds having different media to operate in parallel. Both the filters received same influent.

Laboratory filters were prepared from plexiglass tubes having an internal diameter of 2.6 cm. The use of such a small filter was necessary in view of the high cost and limited supply of latex particles which were used to prepare influent suspensions. It was intended to compare the results of the filtration experiments of this research with those of Habibian (1971). Therefore, it was decided to use more or less the same filter depth and filtration rate that Habibian (1971) employed in his experiments. The filter depth in most of the experiments was 15.0 cm. The use of such a shallow filter in comparison with the 75 cm of bed employed commonly in a conventional rapid sand filter was necessary to get the detectable turbidity in effluent. Moreover, the objective of the experimental investigation was to verify the proposed mathematical model rather than attributing more significance to the extent of removal.

A bed porosity of 0.429 and a filtration rate of 0.136 cm/sec were employed. These values are more or less similar to those used in conventional rapid sand filters.

Glass beads (supplied by Light and Co., Azamgarh, India) were used as filter media. These beads had mean diameters of 0.3 mm and 0.5 mm (data supplied by the manufacturers). These beads were quite uniform and spherical in shape to the extent which can be seen by the microscope (10x). However, in few experiments using clay suspension, sand with Geometric Mean (GM) diameter of 0.297 mm was employed.

The ratio of the diameter of the filter column to the grain diameter was greater than 50 and 85 for 0.5 and 0.3 mm glass beads respectively. It has been reported that wall effects are negligible for values of this ratio greater than 50 (Rose, 1951).

The filters were mounted on wooden frame. A fine brass wire mesh was inserted in the filter bottom to prevent the escape of filter grains. Provision for measuring the head loss across each filter at various depths was made. Polyethylene tube manometers, 0.6 cm in diameter, were used to measure the head loss. Connections were made with rubber tubing. Two manometer lines were connected to dimatrically opposite taps at each level in the filter column opposite taps. This avoided erroneous readings of pressure heads due to air blocks clogging etc. Normally the two manometers gave equal or close readings and in the latter instance a mean value was used. A sampling point at the effluent side of each filter

was provided. A flow meter (Maximum Flow Rate: 84.6 cc/min; Model: 5 GC; supplied by IEPL, Hyderabad, India) was installed on each sampling tube with an accompanying screw clamp to permit the adjustment of the flow. Test tubes, about 20 cc in volume, were used for sample collection.

5.2.2 Preparation of the Filter Bed

Elaborate preparation of the filter beds was required. Everytime the glass beads were first soaked in O.1 N NaOH followed by several washings with distilled water. To alter the zeta potential, filter media was coated with alum as per the procedure described by Sriramulu (1975).

About 275 gm of filter media was taken in a one litre plastic bottle containing 550 cc of 50 mg/lit alum solution and kept on rotating shaker (supplied by Gansons Pvt. Ltd., Bombay, India) at 40 RPM for 1 hr. At this high dose, alum formed micro flocs and coated the media. The media was then carefully transferred into the filter column without agitation. This procedure ensured a uniform coating of filter media.

Water from the clean water overhead tank was then passed through the coated filter beds to permit establishment of the desired rate of flow through the system. This tank was made of plexiglass and equipped with an overflow and two outlets, each connected to one of the filters.

The distilled water containing sodium bicarbonate (10⁻³ M) and sodium chloride (10⁻³ M) was employed to establish the flow. Thus this water resembled the actual influent to the filter with respect to solids concentration, pH and alkalinity.

A small centrifugal pump was used to lift this water to the overhead tank.

After setting the flow, the filter beds were tapped slightly to produce the required filter depth and thus the required bed porosity. Before introducing the suspension into the filters, the "equality" of filter beds so prepared was checked. This was done by the comparison of the ratio Q^{n} . Here, Δh_{0} is the initial head loss across the filter (cm) and Q is the rate of flow through the filter (cc/min). The ratio Δh_{0}^{n} had values of 0.142 and 0.188 for 0.5 mm glass beads at 15.0 and 20.0 cm respectively. The corresponding values for 0.3 mm glass beads were 0.393 and 0.524. If the measured value of Q^{n} for any filter deviated more than Q^{n} 0.005 from the above values, the preparation of that bed was repeated until this criterion was satisfied. In all experiments, the head over the media surface was more or less kept constant at 1.73 \pm 0.01 m during the entire length of the filter run.

5.2.3 Characteristics and Preparation of the Suspension

After completing the preparation of the filter bed and the setting of the flow rate the suspension to be treated could be introduced to the filters. Latex particles (Dow Chemical Co.) with mean diameters of 0.109, 1.1 and 7.6 micron were utilized to make different suspensions. Like most of the colloidal particles found in natural water and wastewater, these latex particles are negatively charged and thus provide a useful model colloidal suspension. Furthermore,

they are very uniform in size (Table 5.1). This uniformity is quite useful in filtration research, because the efficiency of packed bed is quite sensitive to the size of the suspended particles.

m - 1- 3 -	T 4	_			_	*	•
Table	5.1.	Some	properties	~£	1 74 7-4	7)	
		O Child	properties	UL	τ atex	Particles	

THE RESIDENCE OF STANDARDS	ATTACAMENT OF THE A ALC HE TO A SHOWN THE TOTAL A DISK THE A AREA	gen in any sandaren makana ina gy	gan verse nt -
Mean Size, micron	Standard Deviation, micron	No. of Measurements	Density, gm/cc
TOTAL LEGISLATION OF THE STATE	e to an annual communication of the communication o		
0.109	0.0027	318	1.05
1.1	0.0059	106	1.05
7.6	2.3		1.05

^{*} Data supplied by the Dow Chemical Co.

The influent suspension was prepared by proper dilution of concentrated latex suspension. Dilution was accomplished with a distilled water-sodium bicarbonate-sodium chloride mixture identical to that employed for setting the flow.

After equilibration with the laboratory atmosphere the suspensions had a concentration of 10⁻³ M of sodium chloride and sodium bicarbonate and maintained the pH at about 8.5 with an ionic strength similar to that of a typical natural water.

The suspensions of these particles were stored in a 70 litre polyethylene tank prior to use. The contents of this tank were mixed by a heavy duty stirrer (Model Q=1=125, supplied by REMI, Bombay, India) to assure uniform particle

concentration within the entire bulk of the suspension.

In few experiments, kaolinite suspension prepared in the laboratory as per the procedure described by Salome (1980) was used. The ionic strength and pH of this suspension was same as that of latex suspension.

5.2.4 Addition of Destabilizing Agent to the Filter Influents

Because of the nonavailability of Indian made cationic polyelectrolytes and the problems involved in importing such polyelectrolytes, it was decided to use alum as destabilizing agent. GR grade alum (supplied by S.M. Chemicals, Baroda, India) with molecular weight 630.39 and chemical formula ${\rm Al}_2({\rm SO}_4)_3.16{\rm H}_2{\rm O}$ was used. The desired dose of alum was added from the stock alum solution (0.5 percent) prior to pumping the influent suspension.

5.2.5 Measuring the Filter Efficiency

The filter efficiency can be determined by measuring the concentration of suspended particles in the filter influent and effluent. Often the nature and extent of experimentation dictate the method which should be employed for measuring the process variables.

A light-scattering method seemed appropriate. For convenience, optical density was used as an indicator of the amount of light-scattered; a Backman Model DU2 ultravoilet spectrophotometer was employed. For kaolinite suspensions, optical density was measured by spectrophotometer (supplied by Systronics, Ahemdabad, India) at wavelength of 440 mm.

The optical density of latex suspensions with particle sizes 0.109, 1.1 and 7.6 micron were measured at wavelengths of 270, 490 and 790 mm. Calibration curves were prepared by measuring the optical density of the known suspensions at these wavelengths. The curves proved to be linear for the range of concentrations used in this investigation. Accordingly, the ratio of filter effluent to influent optical densities was used in evaluating the filter efficiency. The optical density changes with particle size, thus the existence of particles in the filter effluent which might have grown in size during the course of filtration can reduce the accuracy of the evaluation. However, none of the many microscopic observations made by Habibian (1971) on filter effluents for 1.1 and 7.6 micron latex particles revealed the existence of any particle aggregates. Thus the reported ratio can be considered as the real ratio of particle concentration in filter effluent and influent.

When using 0.109 micron latex, the particles could not be observed using an ordinary optical microscope either in the filter influent or effluent. In view of the very rapid transport of these particles by diffusion, the occurrence of particles aggregate in the filter effluent is theoretically possible. Since such occurrence could increase the optical density (Habibian, 1971), the reported efficiency for 0.109 micron particles can be slightly underestimated.

5.3 Destabilization Experiments

Destabilization experiments were conducted to determine the alum dose to be used in filtration experiments. The idea of using alum was to reduce the surface charge of the particles so as to enhance the particle-to-particle and particle to filter media grain attachment. The procedure used for determining the desired alum dose is described in the following section.

5.3.1 Jar Test

Jar tests were conducted to determine the appropriate alum dose necessary for destabilization of latex and clay particle suspensions. These suspensions were prepared by proper dilution of the concentrated stock suspensions with distilled water. Sufficient sodium chloride and sodium bicarbonate were added to the distilled water to provide a concentration of 10-3 M of each of these substances. The jar test apparatus (supplied by PHIPPS & BIRD Inc., USA) was used for the destabilization experiments. Equal volumes of the suspension to be destabilized were added to each of the six jars used. Appropriate amounts of the alum was then introduced into each jar, while the contents of the jars were rapidly agitated. The rapid stirring at 100 RPM continued for 2 minutes followed by a period of slow stirring at 30 RPM for 20 minutes. The residual light absorption by the suspension after 30 minutes of settling was used as the index of the extent of particle destabilization. The maximum

possible alum dose which did not show any significant difference between initial (prior to addition of alum) and final (after destabilization) light absorption was chosen for destabilization. For each particle size an appropriate wavelength was selected (Section 5.2.5).

6. MODEL VERIFICATION

The success of any mathematical formulation for predicting the dynamic behaviour of deep bed filters depends upon the extent of quantitative agreement between model predictions and the observations made in laboratory and field. Therefore it is essential to verify the proposed model using laboratory and field data on deep bed filtration.

Extensive data on filter performance are available with different sets of operating and system variables. However, the lack of information on particle size distribution stands as a major obstacle in utilizing such data for verifying the conceptually developed formulations for predicting the filter performance. Very few studies are conducted in filtration research controlling the suspended particle size. Habibian (1971) has conducted extensive studies on filtration using different particle sizes in the suspension. Therefore the data presented therein have been exhaustively used to verify the proposed model. Besides some more experiments are conducted in the present research under different set of conditions with special reference to varying suspended particle sizes to check the validity of the model in more realistic situations.

The use of proposed model [Eqs. (4.2) to (4.4), and (4.7)] to describe filter performance requires evaluation of the terms η , η_p , α , α_p , β_c , β_p and β' . The single collector removal efficiency (η α) is calculated from the experimental data for a 'clean' filter, using Eq. (4.4) at t = 0 as follows.

$$\frac{n}{n_{D}} = e^{-\frac{3}{2}\frac{(1-F)}{2}} \cdot L \cdot \eta \alpha$$
 (6.1)

or

$$\eta \alpha = -\ln \left(\frac{n}{n_0}\right) / \left[\frac{3}{2} \cdot \frac{(1-F)}{d_C} \cdot L\right]$$
 (6.2)

Here, L is the depth of the filter bed.

With this initial condition established, the constants $\eta_p \; \alpha_p$, $\beta_c \; \text{and} \; \beta_p \; \text{are computed using non-linear curve fitting techniques. Morquardt (BSOLVE REGRESSION ALGORITHM) is used to solve for the coefficients in multivariable non-linear regression equations (Kuester and Mize, 1973). The details of this algorithm are presented in Appendix B. The values of <math display="inline">\eta$ and η_p are calculated using Happel's flow model (Happel, 1958). The pertinent equations are described as follows.

$$\eta_{\rm D} = 4.04 \, {\rm A_s}^{1/3} \, {\rm P_e}^{-2/3} \tag{6.3}$$

$$\eta_{I} = \frac{3}{2} A_{s} \left(\frac{dp}{dc}\right)^{2} \tag{6.4}$$

$$\eta_G = \frac{(\rho_p - \rho)}{18 \mu V_0} g \cdot d_p^2$$
 (6.5)

and

$$\eta = \eta_D + \eta_I + \eta_G \tag{6.36}$$

Here, η_D , η_I , and η_G represent the dimensionless single collector collision efficiencies when the respective transport mechanisms are diffusion, interception and sedimentation, and

P is the Peclet number given by the following expression.

$$P_{e} = \frac{V_{o} d}{D_{BM}}$$
 (6.7)

and

$$D_{BM} = \frac{kT}{3\pi \mu} \frac{d}{dp}$$
 (6.8)

The computed values of the η_D , η_G , η_I and η for the different set of conditions employed in the verification of the model are presented in Table 6.1. The computed value of η_p using Eqs. (6.3) and (6.4) comes out to be more than 1.0. Since the collision efficiency cannot be more than 1.0, η_p is taken equal to 1.0. The values of α and α_p are computed as follows.

$$\alpha = (\eta \alpha)/\eta \tag{6.9}$$

$$\alpha_{p} = (\eta_{p} \alpha_{p})/\eta_{p} \tag{6.10}$$

The value of β ' is computed using Eq. (4.7) in a similar way to the computation of η_p α_p , β_c , and β_p . The model verification is presented in two different sections using

- 1. The data available in literature,
- and 2. The data obtained in the present investigation.

The validity of the model was checked by the two statistical parameters, the Coefficient of Correlation (R), and the Standard Error of Estimate (S). The expressions for R and S are given in Appendix C. The low value of S together with the value of R approaching the unity is an indication of the good agreement between model predictions and experimental observations.

Table 6.1. Computed collision efficiencies for clean collector using Happel's flow model (Happel, 1958)

Temperature = 300° K; g = 981.0 cm/sec²; ρ = 1.00 gm/cc

and the second s				
d _p ,	η _G	$\eta_{ m I}$	η_{D}	η
1. d _C	= 0.038 cm; F ₀ =			
0.109	0.2357×10 ⁻⁶		0.7980x10 ⁻²	
1.100	0.2400x10 ⁻⁴	0.1655x10 ⁻²	0.1709x10 ⁻²	0.3388×10 ⁻²
7.600	0.1146x10 ⁻²	0.7899x10 ⁻¹	0.4711x10 ⁻³	0.8061x10 ⁻¹
2. d _c	$= 0.03 \text{ cm; } F_0 =$	$0.429; V_0 = 0.$,136 cm/sec; p	= 1.05 gm/cc
0.109	0.2357x10 ⁻⁶	0.1676x10 ⁻⁴	0.8062x10 ⁻²	0.8079×10 ⁻²
1.100	0.2400x10 ⁻⁴	0.1706x10 ⁻²	0.1726×10 ⁻²	0.3457×10 ⁻²
7.600	0.1146x10 ⁻²	0.8146x10 ⁻¹	0.4759×10 ⁻³	0.8308x10 ⁻¹
3. d _c	= 0.05 cm; F ₀ =	$0.429; V_0 = 0.$,136 cm/sec; p _r	= 1.05 gm/cc
0.109	0.2357×10 ⁻⁶	0.6032x10 ⁻⁴	0.5735x10 ⁻²	0.5742×10^{-2}
1.100	0.2400x10 ⁻⁴	0.6143x10 ⁻³	0.1228x10 ⁻²	0.1866x10 ⁻²
7.600	0.1146x10 ⁻²	0.2932x10 ⁻¹	0.3386x10 ⁻³	0.3081x10 ⁻¹
A	COLOR DE LA COLOR DE LA CALLE DE COLOR DE CALLE DE CAL	CERTAIN TO THE REPORT OF THE WORLD	The state of the s	

6.1 Model Verification Using the Data Available in Literature

As stated earlier, only Habibian (1971) has conducted filtration experiments controlling physical and chemical parameters influencing the filtration process with particular reference to the size of the suspended particles, and hence his data is extensively used for the verification of the proposed model.

In one experiment, Habibian operated four identical filters ($d_c = 0.038$ cm, F = 0.36, L = 14.0 cm) at a flow rate of 0.136 cm/sec ($4.8 \, \text{m}^3/\text{m}^2/\text{hr}$), filtering a suspension of latex spherical particles ($n_c = 11.0 \, \text{mg/lit}$, $d_p = 0.109 \, \mu\text{m}$, $\rho_p = 1.05 \, \text{gm/cc}$). Filter media were coated with cationic polymer prior to use, and polymer was added continuously throughout the runs at a dosage selected to maximize particle—to—particle attachment. Coagulation within the pores of the filter bed was reported to be insignificant. Experimental results of the four runs were similar; these have been averaged and plotted in Fig. 6.1.

The single collector removal efficiency ($\eta\alpha$) is calculated from the experimental data for a 'clean' filter. For example, $n/n_0=0.6$ for the filters in Fig. 6.1. Hence, using Eq. (4.4) at t = 0, $\eta\alpha=1.44298\times 10^{-3}$. With this initial condition established, the constants η_p α_p , β_c , β_p , and β' are determined using non-linear curve fitting techniques. The values of η_p α_p , β_c , β_p , and β' are 0.041, 0.89, 0.13 x 10⁻⁶ and 0.22 respectively. Thus α and α_p can be computed as 0.171 and 0.041 respectively.

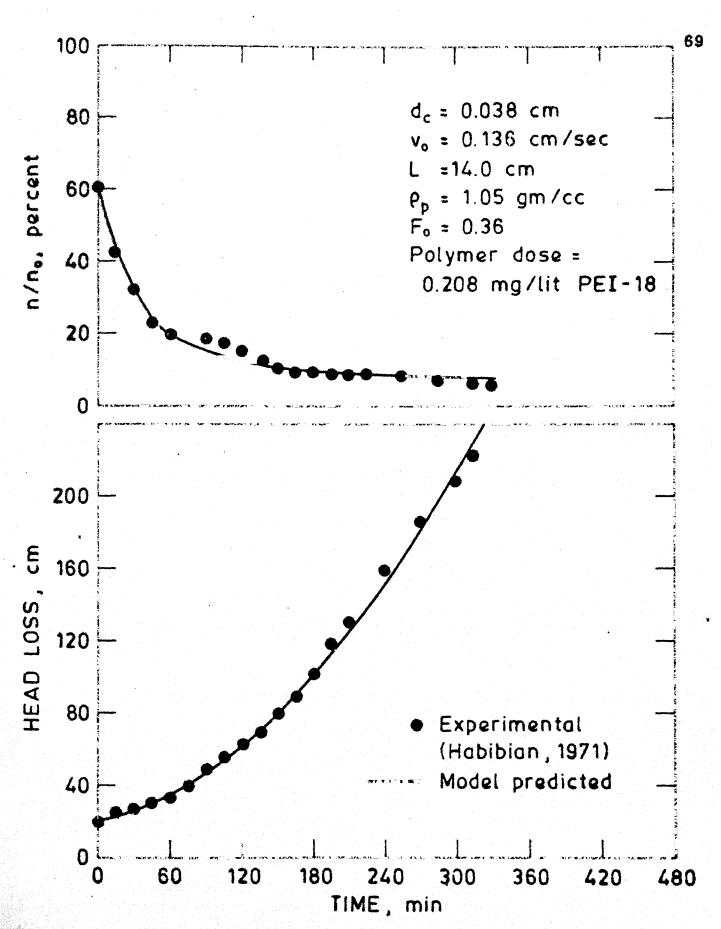


Fig. 61. Model verification ($n_0 = 11.0 \text{ mg/lit}$; $d_p = 0.109 \mu \text{m}$)

Both experimental observations and the model predicted values are depicted in Fig. 6.1 which indicate a very good quantitative agreement between experimental results and model predictions. The values of S and R for the n/n are 1.89 and 0.99 respectively. The corresponding values for the head loss are 4.07 and 0.99 respectively.

The model is further verified using data from other experiments by Habibian (1971) in which one or more filtration variables were significantly different from conditions described in Fig. 6.1. Observed values of the particle removal by the clean filters were used to calculate $\eta\,\alpha$ for each run. Coefficients $\beta_{\rm C}$, $\beta_{\rm p}$, and β' are kept constant as they are not expected to vary significantly with surface properties of the media and particle, and concentration of particles. The value of $\eta_{\rm p}$ $\alpha_{\rm p}$ was estimated for the best fit of the experimental results as it would vary with the surface properties of the media, suspended particles, and size of the suspended particles.

Data from six filtration experiments using three suspended particle sizes, five influent concentrations, and two bed depths are presented in Figs. 6.2 to 6.4. The model predictions are also shown in these figures indicating a very good quantitative agreement with the experimental results. The respective $\alpha_{\rm p}$ values and the corresponding S and R values are presented in Table 6.2. These values also justify the good correlation between experimental values and model predictions in most of the situations.

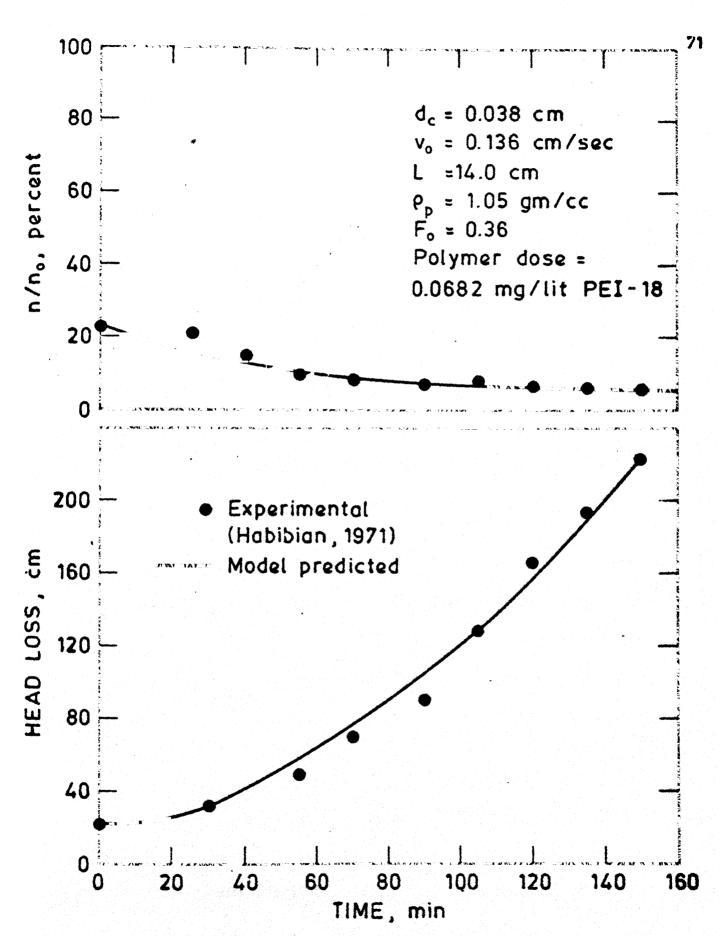


Fig. 6.2. Model verification ($n_o = 9.7 \text{ mg/lit}$; $d_p = 0.109 \mu m$)

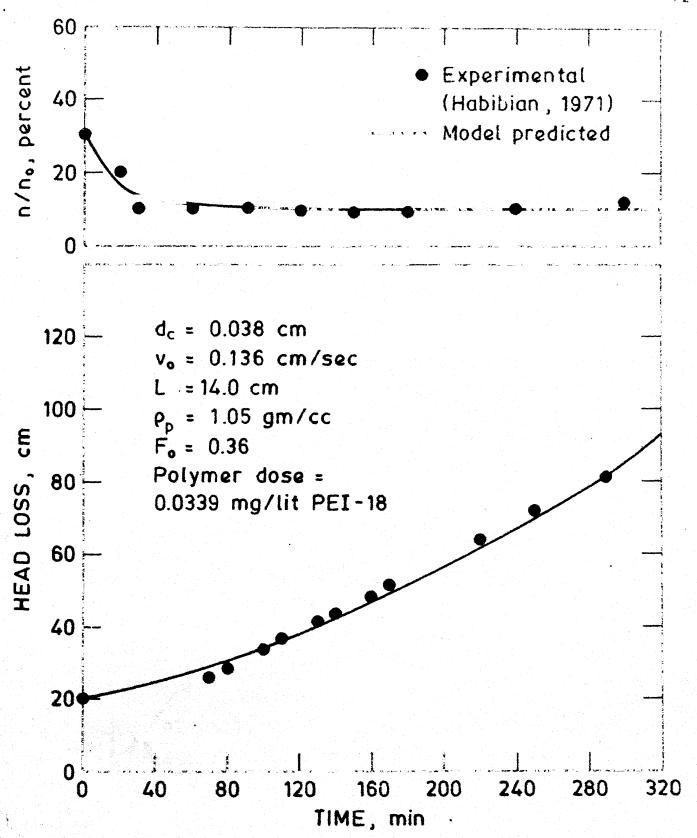


Fig. 6.3. Model verification ($n_o = 37.2 \text{ mg/lit}$, $d_p = 1.1 \mu\text{m}$).

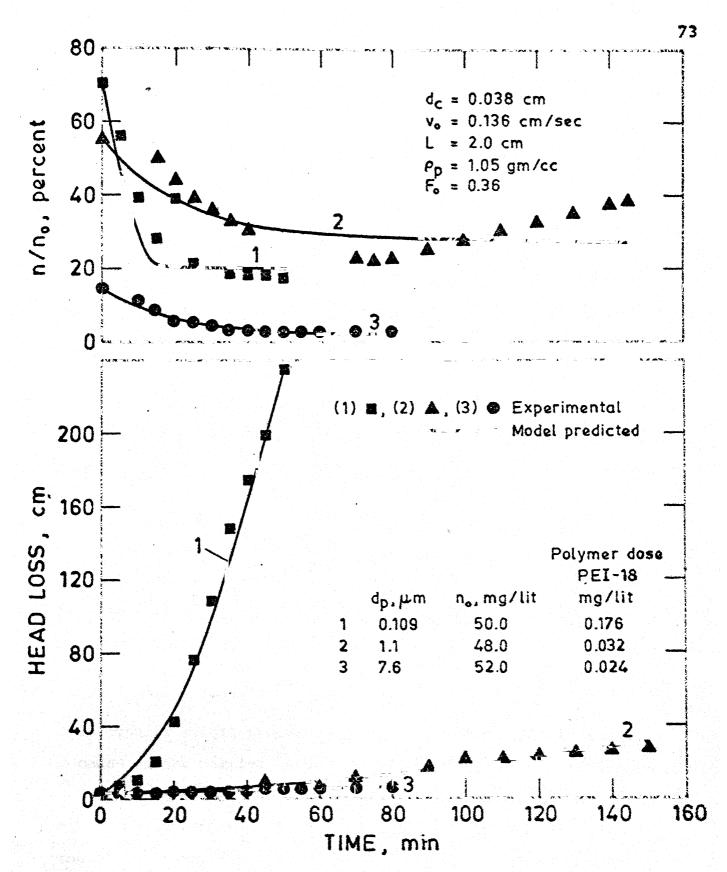


Fig. 6.4. Model verification for particle sizes in the different regions of filtration.

Table 6.2.	Computed	values of	α	and statistical parameters fo	r
			1-	literature	

Fig.	\cdot : u_r			d Error of ce (S) for	Coefficient of Correlation (R) for	
Marini ye kalimi	μm	The Market	n/n _o	Head loss	n/n	Head loss
6.1	0.109	0.041	1.89	4.07	0.99	0.99
6.2	0.109	0.042	2.02	8.26	0.96	0.99
6.3	1.100	0.140	2.54	2.51	0.94	0.99
6.4	0.109	0.041	3.25	1.96	0.89	0.95
6.4	1.100	0.065	7.50	2.33	0.73	0.97
6.4	7.600	0.173	0.95	0.22	0.97	0.97

It is important to note that the α_p value increases with the increase in suspended particle size (Table 6.2). In other words, one may write

$$\alpha_{p} \quad \alpha \quad (d_{p})^{m_{1}}$$
 (6.11)

Here, m₁ is a constant.

This type of relationship of α_p with d_p is generally expected because as the particle size decreases, the charge on the particle surface increases. The increase in particle surface charge increases the thickness of the electrical double layer and hence the energy barrier for successful attachment of the two particles which leads to decrease in α_p value. This observed relationship

of α_p with suspended particle size gives an additional verification of the model since it is able to compute α_p values in accordance with the expected variation of α_p with d_p .

6.2 Model Verification Using the Data Obtained in Present Investigation

The experimental investigation was carried out to supplement the data available in literature on deep bed filtration controlling the suspended particle size to check the validity of the proposed model under different sets of operational and system variables.

The major difference between the experimental investigation of Habibian (1971) and that of the present study is the use of alum as destabilizing agent instead of polyelectrolytes. The second significant difference is the initial bed porosity and the use of two different media sizes.

The data from three filtration experiments employing three different suspended particle sizes, viz., 0.109 μ m, 1.1 μ m, and 7.6 μ m, are presented in Figs. 6.5 to 6.7. The model predictions are also shown on these figures indicating a very good quantitative agreement with the experimental results. The respective α_p values and the corresponding values of the statistical parameters are presented in Table 6.3.

It is interesting to note from Figs. 6.5 to 6.7 that even though the initial bed porosity is same with 0.03 and 0.05 cm media sizes, the initial head loss, particle removal, and the head loss development patterns are quite different. This clearly indicates that the surface area and the individual pore sizes

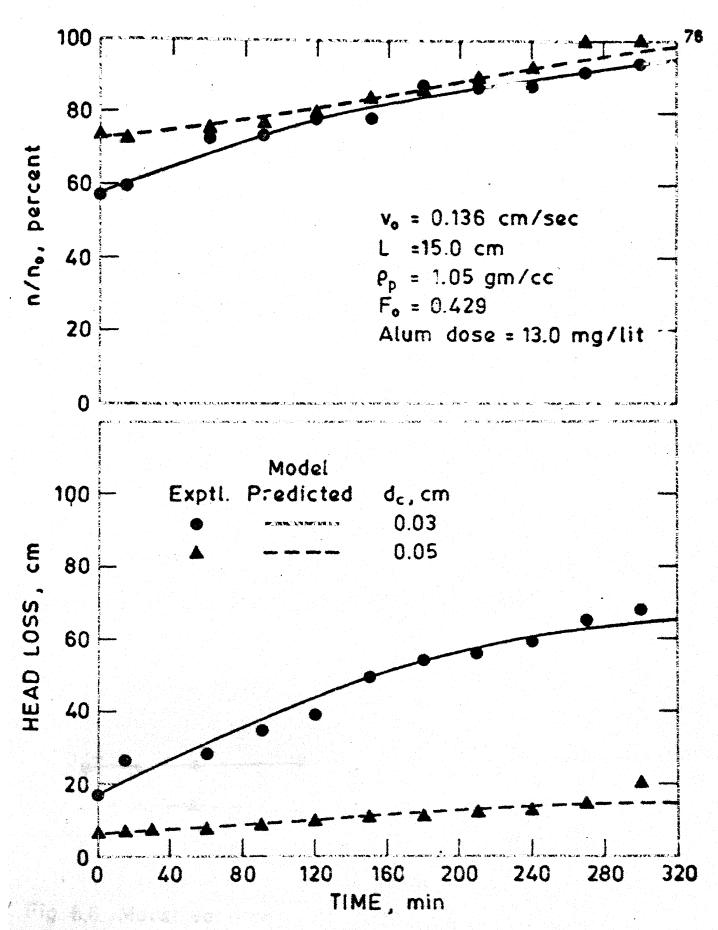


Fig. 6.5. Model verification ($n_0 = 20.0 \text{ mg/lit.} d_p = 0.109 \mu m$)

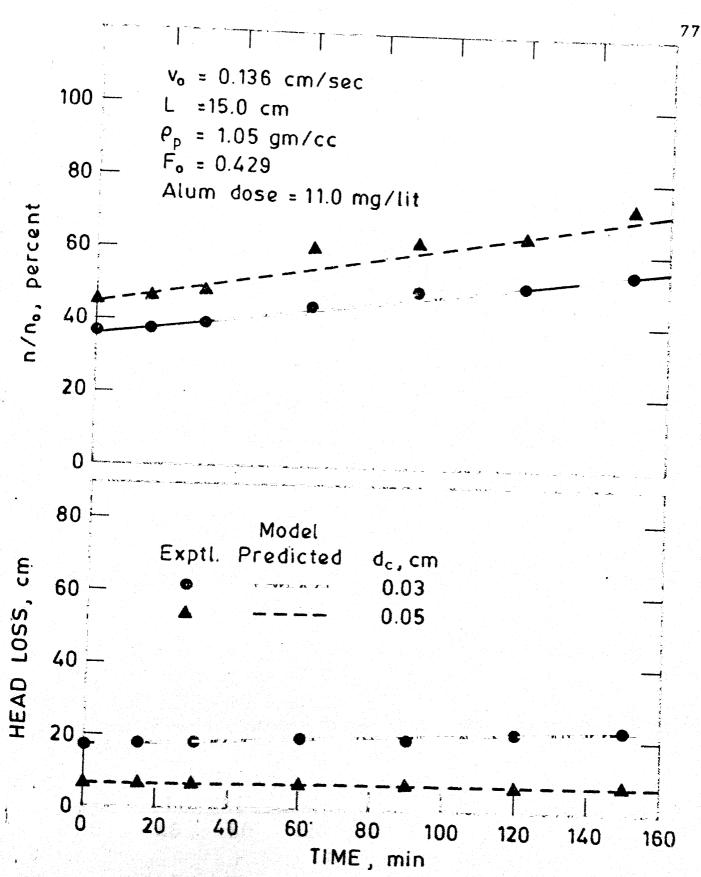


Fig. 6.6. Model verification ($n_0 = 20.0 \text{ mg/lit}$, $d_p = 1.1 \mu \text{m}$)

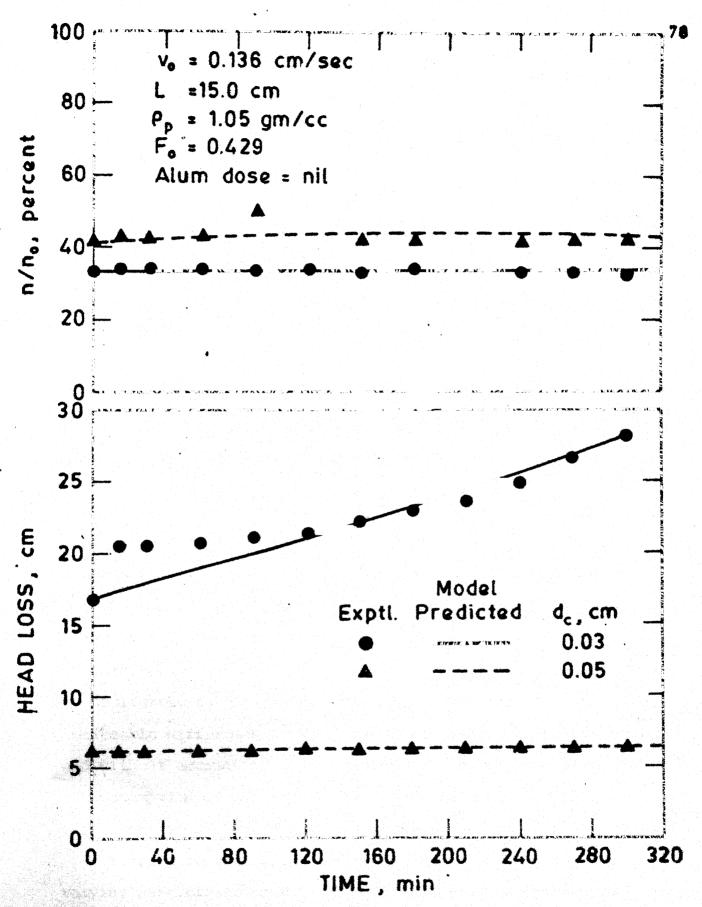


Fig. 6.7. Model verification ($n_0 = 40.0 \text{ mg/lit}$, $d_p = 7.6 \mu \text{m}$)

Table 6.3. Computed values of α_p and statistical parameters for the data obtained in present investigation

Fig.	d _p	α_{p}	Standard Error of Estimate (S) for		Coefficient of Correlation (R) for	
AMERICAN STRUCTURE OF THE STRUCTURE OF T	μm	I I I I I I I I I I I I I I I I I I I	n/n	Head loss	n/n	Head loss
6.5	0.03	0.019	2.96	7.77	0.99	0.92
6.5	0.05	0.019	17.42	1.86	0.64	0.90
6.6	0.03	0.020	1.65	0.72	0.99	0.97
6.6	0.05	0.021	4.11	0.07	0.98	0.98
6.7	0.03	. 0.023	8.39	1.47		0.96
6.7	0.05	0.022	15.20	0.09		0.47

Furthermore, as the filtration than the initial bed porosity. Furthermore, as the filtration progresses the change in surface area of the media and the individual pore size are mainly responsible in head loss development than the decrease in bed porosity. This is because the computed changes in the bed porosity (Eq. (4.10)) as the filter run progresses are found to be negligible in all the experiments. Hence there was no noticeable difference in model predicted filter performance with and without accounting for the variation in bed porosity. Thus the assumption of constant bed porosity is quite justified in the filtration of water and wastewater.

To be more realistic, the model should be verified for varying particle sizes in the influent. In order to achieve this,

experiments were conducted with different combinations of the three available latex particle sizes, viz., 0.109 μm , 1.1 μm , and $7.6 \ \mu\text{m}$. The total influent particle concentration was kept constant in all such experiments. The main difficulty in these experiments was to estimate the effluent quality. Many attempts were made to estimate the concentration of different particle sizes in the effluent, but none of these were successful. only method available to estimate the particle size distribution is with the use of Particle Counters. This method could not be used because of the non availability of Particle Counter. Therefore validity of the model could be checked only for the head loss data. The results of the four filtration experiments conducted with different combinations of latex particles are presented in Figs. 6.8 to 6.11. The model predicted head loss values are in good agreement with the experimental observations indicating the validity of the model even with varying suspended particle sizes in the filter influent. However, the definite conclusion in this regard can be drawn only when the experimental observations confirm the model predictions for effluent quality also.

6.3 Filtration of Clay Suspension

Filtration experiments with clay suspension using glass beads and sand as filter media were conducted with two main objectives

to compare the filtration performance of two media,
 viz., glass beads and sand, and

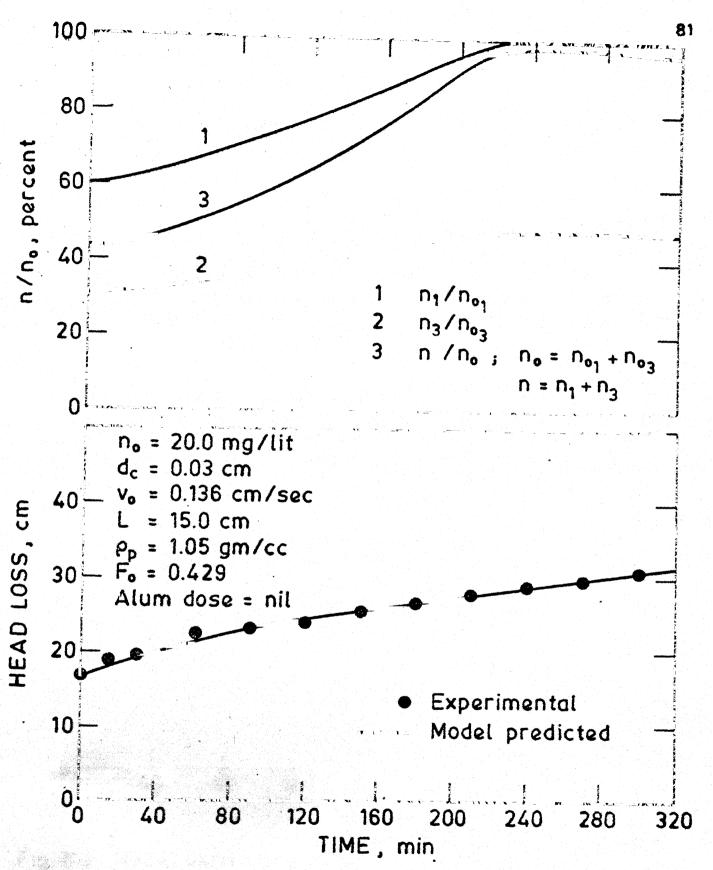


Fig. 6.8. Model verification $(d_{p_1} = 0.109 \, \mu m$, $n_{e_1} = 10.0 \, mg/lit$; $d_{p_3} = 7.6 \, \mu m$, $n_{e_3} = 10.0 \, mg/lit$).

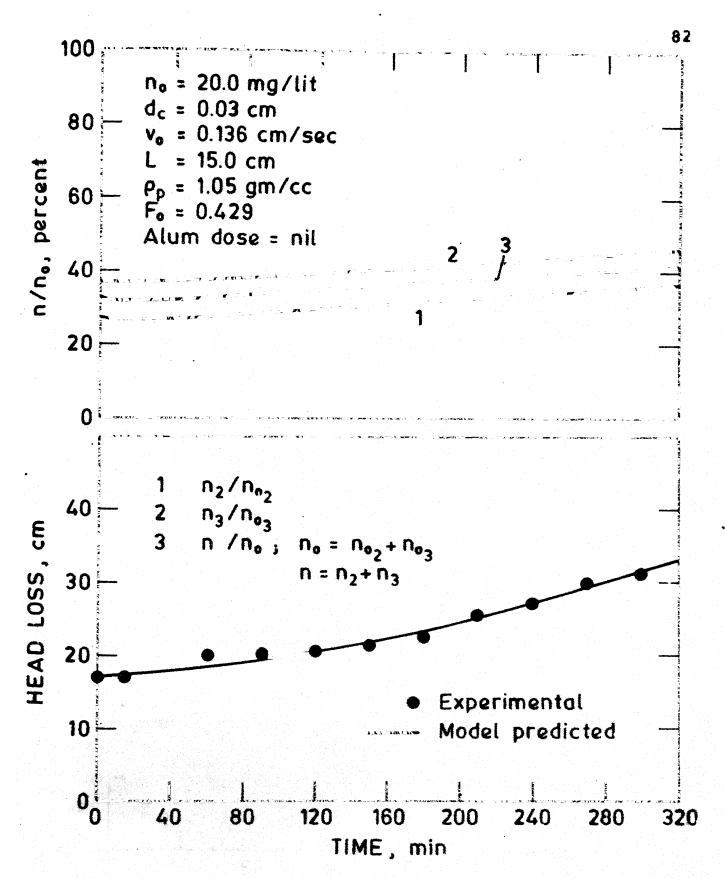


Fig. 6.9. Model verification ($d_{p_2} = 1.1 \,\mu\text{m}$, $n_{o_2} = 10.0 \,\text{mg/lit}$; $d_{p_3} = 7.6 \,\mu\text{m}$, $n_{o_3} = 10.0 \,\text{mg/lit}$)

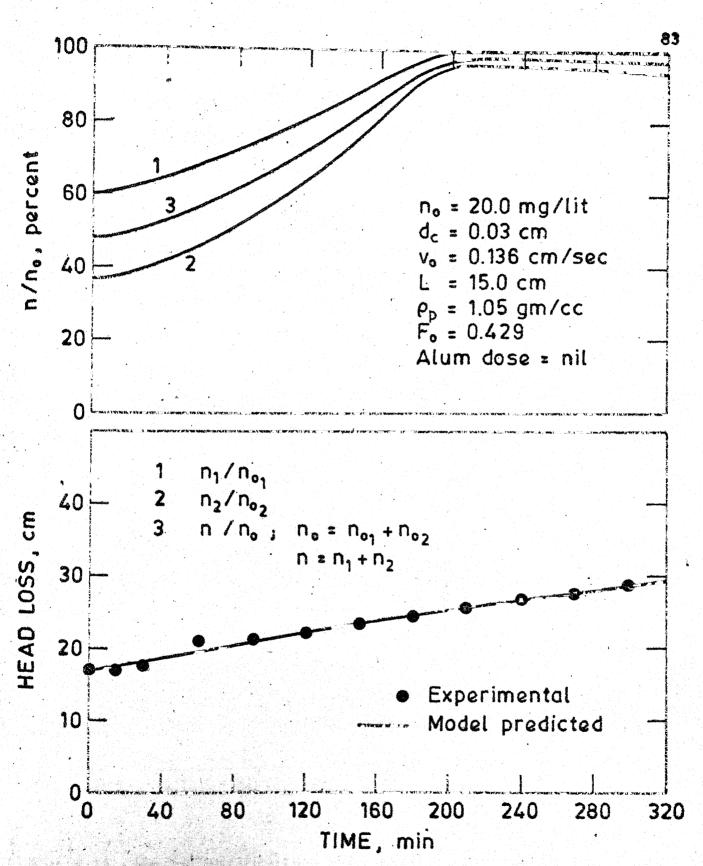


Fig. 6.10. Model verification $(d_{p_1} = 0.109 \mu m, n_{e_1} = 10.0 \text{ mg/lit};$ $d_{p_2} = 1.1 \mu m, n_{e_2} = 10 \text{ mg/lit}.$

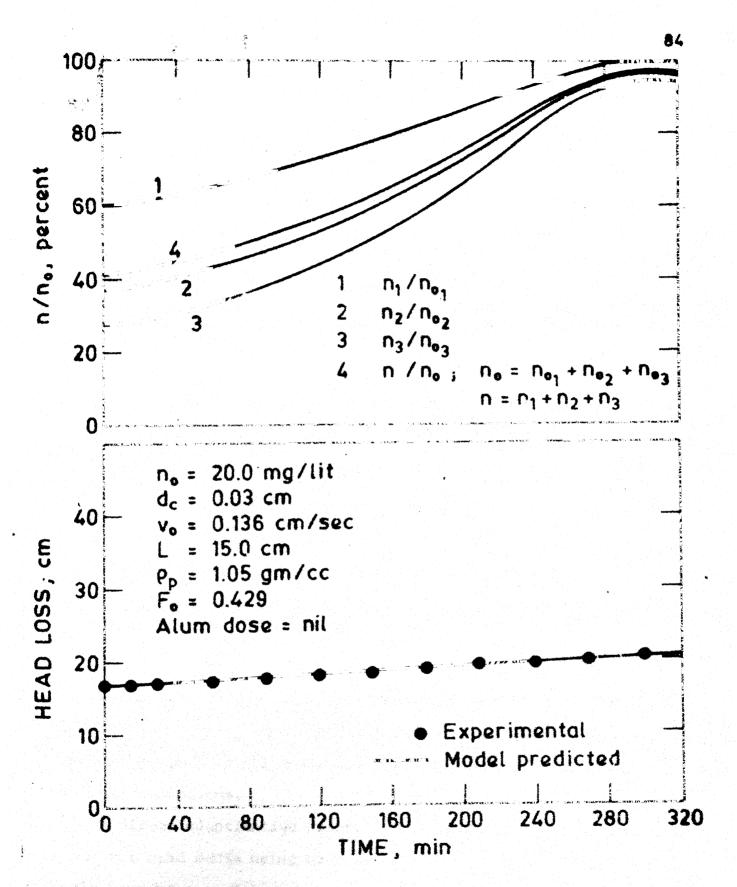


Fig. 6.11. Model verification $(d_{p_1} = 0.109 \,\mu\text{m}, n_{e_1} = 6.65 \,\text{mg/lit}; d_{p_2} = 1.1 \,\mu\text{m}, n_{e_2} = 6.7 \,\text{mg/lit}; d_{p_3} = 7.6 \,\mu\text{m}, n_{e_3} = 6.65 \,\text{mg/lit})$

2. to compare the filtration of latex suspension with clay suspension.

The main differences between the sand media and glass beads media were the initial bed porosity and sphericity of the particle. The initial bed porosity of the sand bed was 0.467 while that of glass beadsbed was 0.429. The major difference between the latex suspension and clay suspension is that the latex particles are exactly spherical and have a particle density of 1.05 gm/cc while clay particles are expected to be flaky and have a particle density of 2.65 gm/cc.

Many experiments were conducted with clay suspension using glass beads (0.03 cm and 0.05 cm) and sand (0.03 cm GM), and varying physical and physico-chemical parameters influencing filtration. The results of one such typical experiment are presented in Fig. 6.12. Qualitatively both sand and glass beads behave in a similar way. This indicates that the proposed model could as well be valid for sand media which is very commonly used for filtration of water and wastewater, only the model parameters $\beta_{\rm C}$, $\beta_{\rm p}$, and $\beta^{\rm t}$ would be different. Similarly the compassion of the filtration of clay suspension and latex particles (Figs. 6.5 and 6.12) shows a qualitative agreement. This would mean that the proposed model could also be applied to the filtration of clay suspensions.

A direct quantitative proof of the validity of the proposed model for sand media using clay suspension was necessary and would have been much more convincing to accept the model. Again,

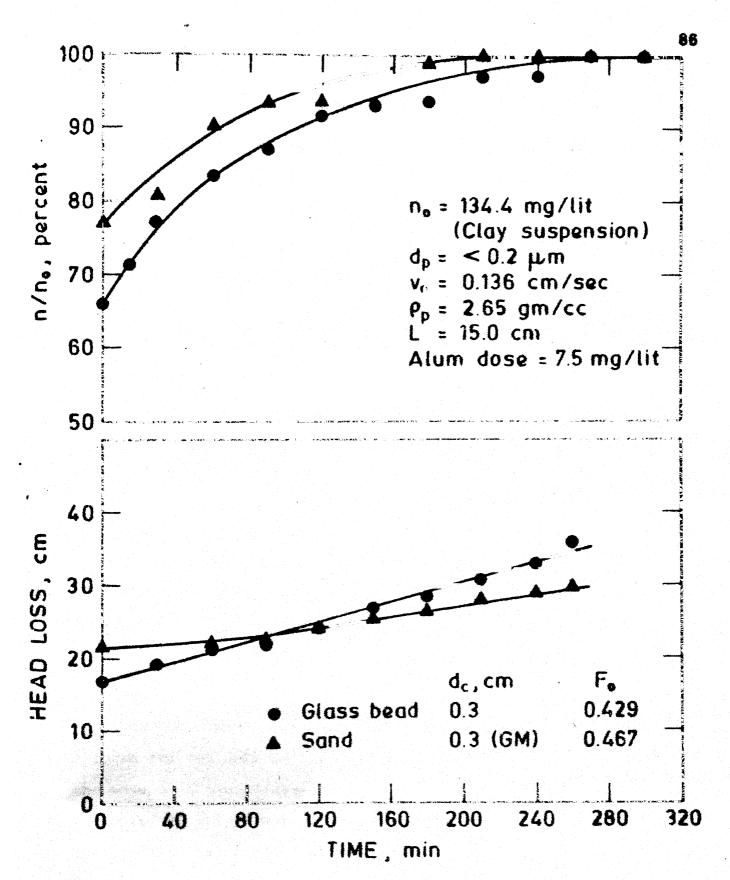


Fig. 6.12. Filtration of clay suspension using glass beads and sand as media.

unfortunately the lack of particle size distribution data limits the present study to give only a qualitative validity of the model in such conditions.

6.4 Variation of Particle-to-Particle Attachment Coefficient

Particle—to-particle attachment coefficient (α_p) would mainly depend upon the surface properties, particularly the surface charge of the particles. The particle surface charge may be expressed in terms of zeta potential of the particles. In other words, α_p can be related to zeta potential. In coagulation and filtration the zeta potential is controlled by the addition of destabilizing agents such as bi—and multi-valent cations, polyelectrolytes etc. It would be very much useful if a relationship between α_p and the zeta potential can be developed. However, non existence of sufficient data about filtration efficiency controlling both particle size and zeta potential limits the development of such a quantitative relationship.

Presently an attempt has been made to empirically correlate α_p with polyelectrolyte dose which in turn controls the zeta potential. The data of Habibian (1971) have been used for this purpose.

The computed α_p values are plotted with polyelectrolyte dosages for two different particle sizes in Fig. 6.13. Noting the nature of the variation of α_p with polyelectrolyte dosage an empirical relation is proposed relating these two variables. The equation is of the following form

$$\operatorname{Ln} \ \alpha_{p} = -(\mathbf{A}_{1} \ \mathbf{x}^{2} + \mathbf{A}_{2} \ \mathbf{x} + \mathbf{A}_{3}) \tag{6.12}$$

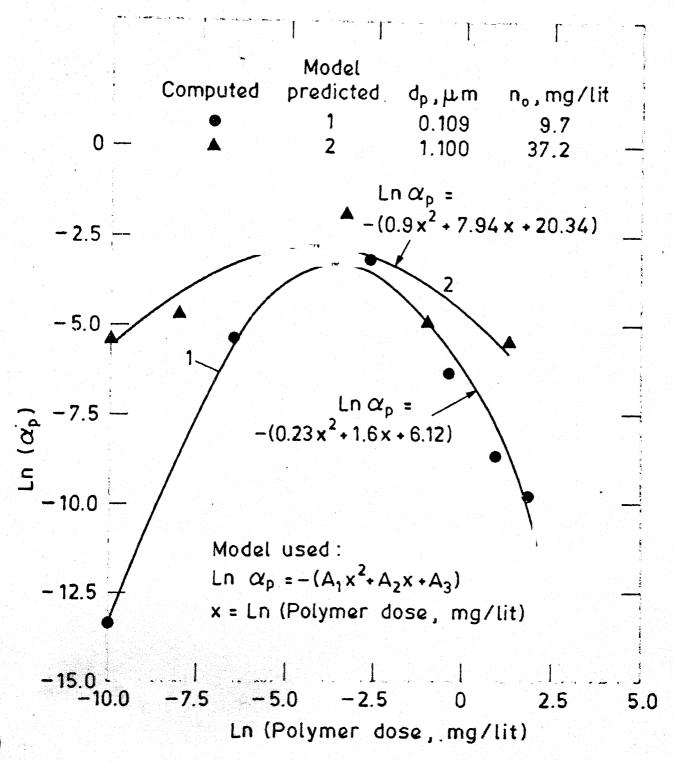


Fig. 6.13. Variation of particle-to-particle attachment coefficient with polymer dose.

Here, x = Ln (Polymer Dosage, mg/lit), and A_1 , A_2 and A_3 are empirical constants.

Obviously, one would expect A₁, A₂, and A₃ to depend upon the particle concentration, suspended particle diameter and surface charge of the particle.

Fig. 6.13 clearly indicates that $\alpha_{\rm p}$ is more sensitive to the polymer dosage for suspended particle size of 0.109 $\mu \rm m$ compared to that of the 1.1 $\mu \rm m$. Hence it is more important to control the polymer dosage when filtering a suspension of lower particle size, i.e., submicron particles compared to the filtration of suspension having higher particle size. Thus the knowledge of particle size can help even in controlling the dosages of destabilizing agents.

7. SIMULATION

Simulation assumes that the system can be described in terms acceptable to a computing system. In this regard, a key concept is that of a "system state description". If a system can be characterized by a set of variables, with each combination of variable values representing a unique state or condition of the system, then manipulation of the variable values simulates movement of the system from state to state. Precisely the simulation is the representation of the dynamic behaviour of the system by moving it from state to state in accordance with well defined operating rules.

With the aforementioned concept of simulation, the deep bed filtration can be simulated by experimenting on a verified proposed model for different combinations of various physical and physico-chemical parameters influencing water and wastewater filtration. In general, the simulation procedure involves the prediction of the dynamic behaviour of

- 1. the system performance, and
- 2. the system state description.

In the present context, the system performance refers to the filter performance which includes filtrate quality and head loss. The system state description refers to the state or condition of the filter bed which in turn gives the clogging picture of the filter bed. The simulation of filter performance and the state of the filter bed are described in two separate sections.

7.1 Simulation of the Filter Performance

The variables influencing filtration may be classified in two groups, viz. physical parameters and physico-chemical parameters. The physical parameters include suspended particle concentration, density and size, media size, porosity, flow rate, and filter bed depth. The physico-chemical parameters include particle-to-media grain attachment and particle-to-particle attachment. The simulation of filter performance for all these parameters is described as follows

Suspended Particle Concentration: The predictions of effluent quality and head loss for four different influent suspended particle concentration are presented in Fig. 7.1. the beginning of the filtration, removal efficiency and head loss are independent of particle concentration as it is not expected to play any role initially, and hence properties of the filter bed and suspended particles will govern the filtration and not the concentration of particles in influent. However, the dynamics of filtration completely changes with the particle concentration. As particle concentration increases removal efficiency increases because of the increasing number of retained particles acting as collectors. After some time the filtration efficiency attains a saturation value because of the surface coverage of the media grains and retained particles acting as collectors. A dynamic equilibrium may be achieved as the new contact sites are not effectively increased and is influenced by the particle concentration. As expected, head loss development

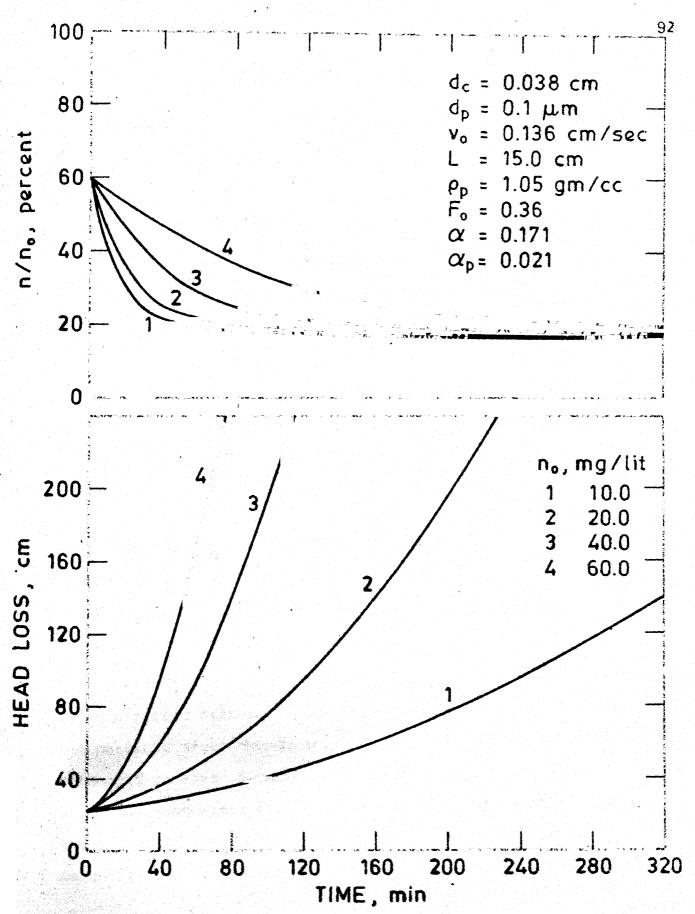


Fig. 7.1. Influence of influent particle concentration on filter performance.

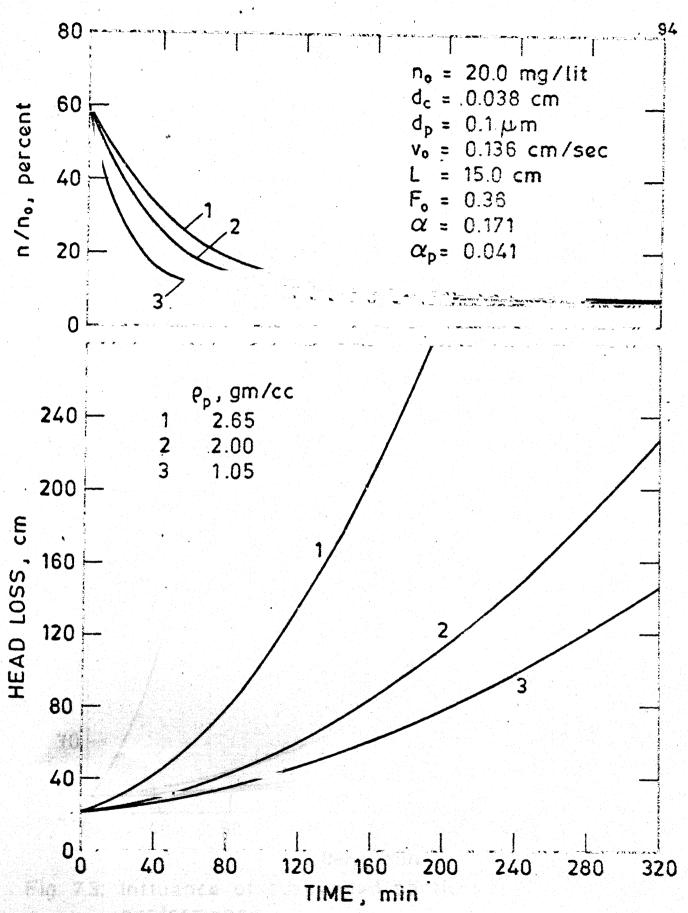


Fig. 7.2. Influence of suspended particle density on filter performance.

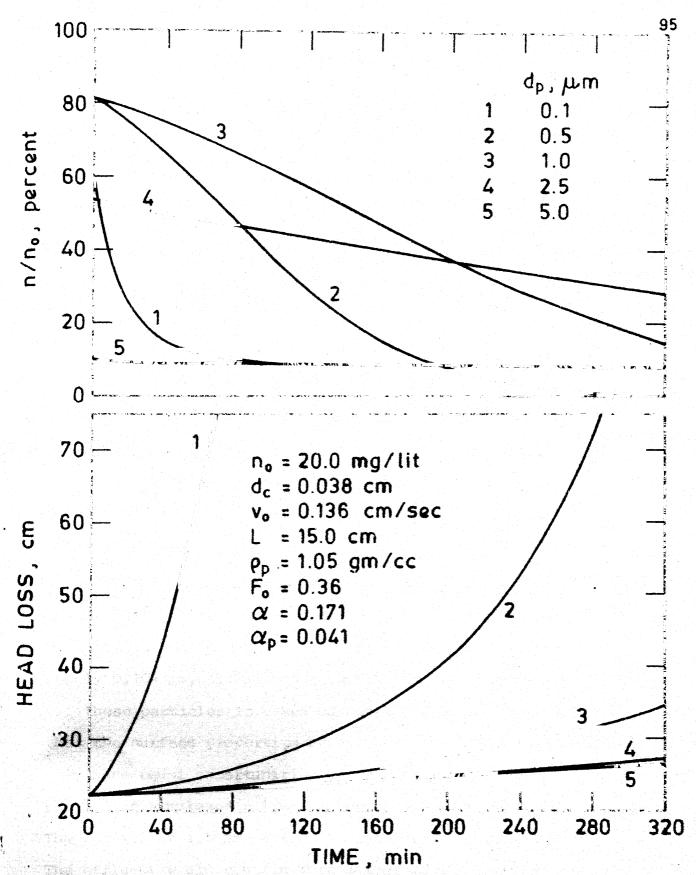


Fig. 7.3: Influence of suspended particle size on filter performance.

removal at the onset of filtration. This is in accordance with the observations of Yao et.al. (1971). Further, one micron particles are the most difficult to remove as the filter run progresses. This is because the rate of increase of retained particles acting as collectors is very slow when only 1.0 micron particles are present. Submicron particles give better efficiency as they can be effectively transported by Brownian diffusion. These particles produce very high head loss because of their more surface area per unit weight of the material removed as compared to bigger particle sizes. The bigger particles (5.0 μm) show more removal as they can be very easily transported by interception and gravity settling. Further, because these particles have low surface area per unit weight of the material removed, the head loss development is not significant. This is in accordance with the experimental observations of Habibian (1971), and that of the present investigation.

D. Varying Suspended Particle Size in Influent: In order to simulate the filter performance in more realistic cases, the influent is considered to have three different particle sizes namely 0.109 μ m, 1.1 μ m and 7.6 μ m. The mass concentration of all these particles is taken as same. It is further assumed that the surface properties of all these particles are such that they have equal opportunities for successful contacts. The results of simulated filter performance are presented in Fig. 7.4. The removal of 1.1 μ m particles continues to pose a problem. The effluent would contain more number of 1.1 μ m particles

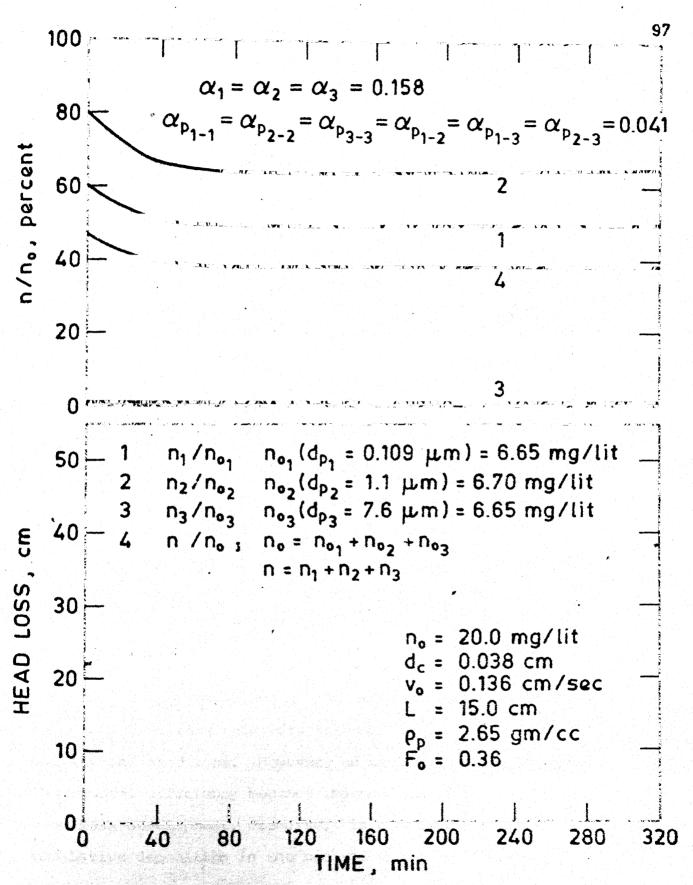


Fig. 7.4. Influence of varying particle sizes in suspension on filter performance.

compared to 0.1 μm particles. The 7.6 μm particles would be removed almost completely. In general it may be said that the filtered effluent would always have major fraction of particles around 1.0 μm size. The head loss development is a direct consequence of the extent and the type of particles removed.

- E. Media Size: Computations illustrating the effects of media size on filtration are presented in Fig. 7.5. As expected, both removal efficiency and head loss increase with the decrease in media size initially as well as with time. Though, media size affects the filter performance, it can be easily measured and readily controlled, and hence is not of major importance.
- F. Clean Bed Porosity: The simulated filter performance for four different clean bed porosities is presented in Fig. 7.6. It is interesting to note that the head loss build-up increases drastically with decreased clean bed porosity whereas the removal efficiency is not affected to that extent. This is essentially because of the more uniform distribution of particles with depth (Refer Part C. Section 7.2).
- G. Flow Rate: Flow rate is an important operational variable to be controlled in filtration process. As is clear from Fig. 7.7, flow rate affects both the initial filtrate quality and head loss. However, as the filtration progresses the removal efficiency becomes independent of flow rate. The head loss development, ofcourse, is a direct consequence of the cumulative deposition in the bed and the flow velocity.

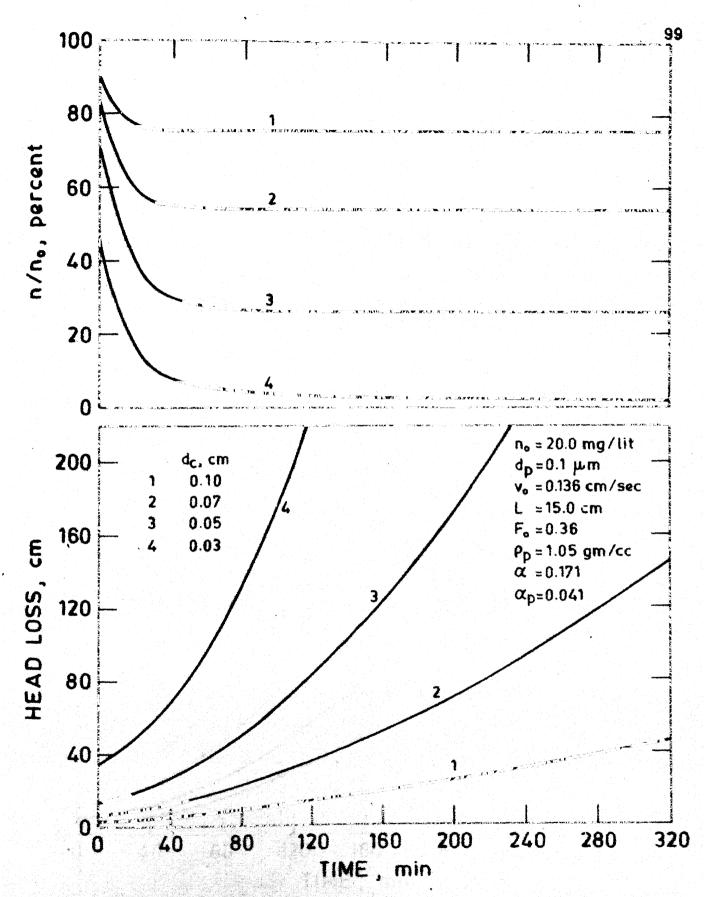


Fig. 7.5. Influence of media size on filter performance.

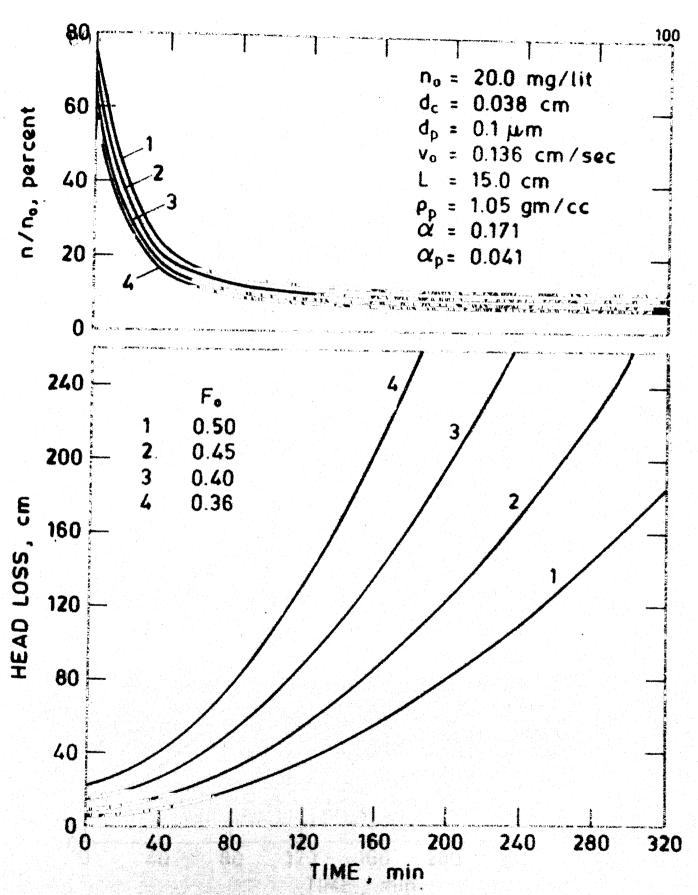


Fig. 7.6. Influence of clean bed porosity on filter performance:

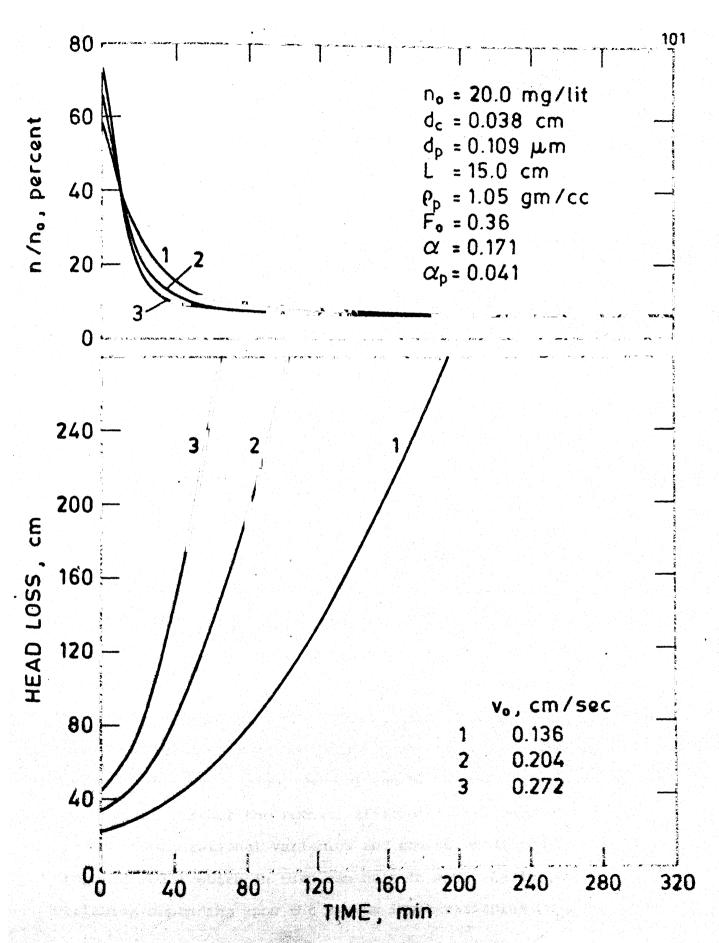


Fig 7.7. Influence of flow rate on filter performance.

Filter Depth: The effects of filter depth and filtration time are illustrated by the simulation results presented in Fig. Removal is distributed throughout the filter bed at the onset of filtration, but becomes localized in the upper regions of the bed as filtration proceeds. Head loss follows a similar distribution. Retained particles accumulate in the upper regions of the bed and lead to the retention of more particles in that zone. A good filter is one which would give uniform removal and head loss with depth. This can be achieved by properly controlling the system and operational variables in filtration. For example, the uniform removal with depth can be achieved by providing larger sized media with lower specific gravity at the top and smaller media with higher specific gravity at the bottom (mixed media) or by adopting upflow filtration. These observations clearly justify the superiority of multi media filters over single media filters. The rate at which the retained particles would increase is dependent on the media size. If the media size is large at the top it will give lower removal at the top and hence the particles are forced to penetrate deep where the media size is low. At lower depths, though the media size is low, because of the low particle concentration at that depth, the rate of accumulation of retained particles is also low. Thus by adjusting the media size, removal can be distributed throughout the depth. Further the removal efficiency will vary with other system and operational variables and can be predicted from the proposed model which in turn can help in manipulating these variables depending upon the system input variables (n_D , d_D ,

led describilities of particles

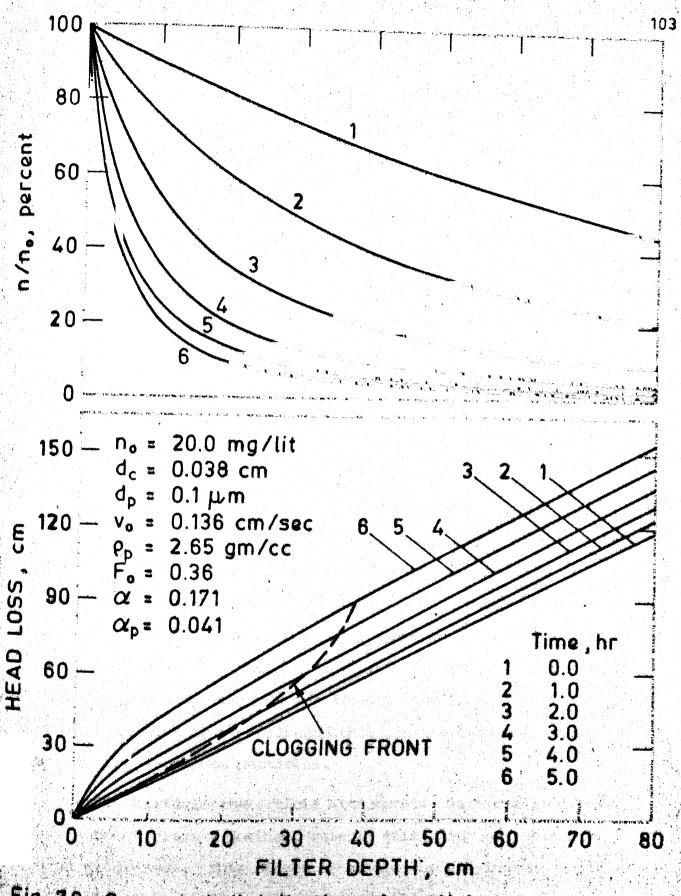


Fig. 7.8. Computed distribution of particle removal and head loss with filter depth.

- $\epsilon_{\rm p}$, $\alpha_{\rm r}$ and $\alpha_{\rm p}$) and the output requirements.
- Particle-to-Media Grain Attachment: The effect of particle-to-media grain attachment on filter performance is depicted in Fig. 7.9. This is achieved by varying the coefficient ' α ' in a simulation model which is a reflection of the particleto-media grain attachment. Initially the removal increases with increase in α value. However, as the filtration progresses, the removal efficiency might increase or decrease depending upon the This is because as the filtration progresses the media grain gets covered due to deposition of particles and the properties of the deposited particles control the attachment step. Depending upon the relative magnitude of the decrease in η_{r} value due to surface coverage and the increase in η_r value due to the retained particles acting as collectors the overall removal efficiency may increase or decrease. The particle-to-media grain attachment (α) is an important parameter and can be controlled by controlling the media and particle properties by giving proper pretreatment either to media or suspended particles or both. This is normally achieved by giving precoat to the media and adding polyelectrolytes to the suspensions or by giving different pretreatments to the filter influent. The major factors which are expected to have influence on α are the zeta potentials of media and suspended particles.
- J. Particle-to-Particle Attachment: Particle-to-particle attachment plays a dominant role in filtration as the filter run progresses. This effect is studied by varying the coefficient α in a simulation model. The results are presented in

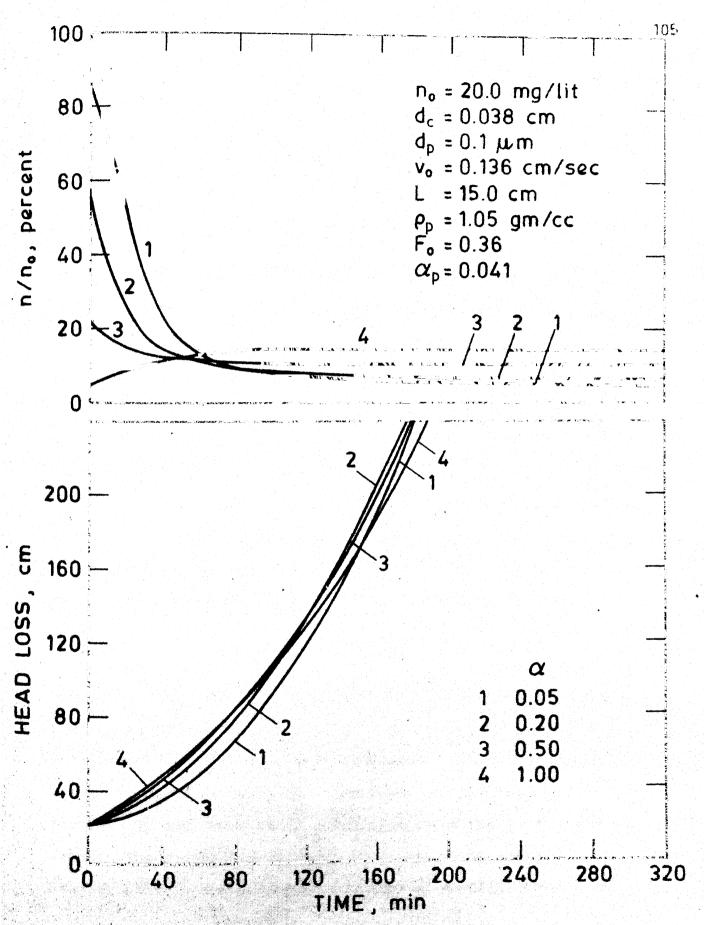


Fig. 7.9. Influence of particle-to-media grain attachment on filter performance.

Fig. 7.10. If $\alpha_{\rm p}$ is zero, i.e., there is no particle-to-particle attachment, then the filter efficiency would continuously decrease because no retained particles would act as collectors and at the same time these retained particles would cover the surface area of the media thereby decrease the particle-to-media grain attachment and hence the overall removal efficiency. As $\alpha_{\rm p}$ increases, the removal efficiency as well as the head loss increase significantly with time. On the other hand, the particle-to-particle attachment does not have any effect on the removal efficiency of clean filters.

7.2 Simulation of the State of Filter Bed

The retention or deposition of the suspended particles as the filtration progresses results in the change of the condition or state of the filter bed These changes are indirectly reflected by the output variations characterized by the filter performance. In order to optimize the filter response for the different sets of input conditions it is necessary to choose the appropriate values of the operational and system variables. In this respect the dynamic changes of the state of the filter bed can play an important role. The filter state may be characterized by the clogging zone. This corresponds to that portion of the filter bed which contributes for the head loss build-up. The depth of this zone changes as the filtration progresses, and at any time (t) after the start of filtration the depth of clogging zone is governed by the depth of floc penetration or the depth of clogging front. The concept of clogging front was first introduced by Stanley (1955), and latter on employed by several investigators

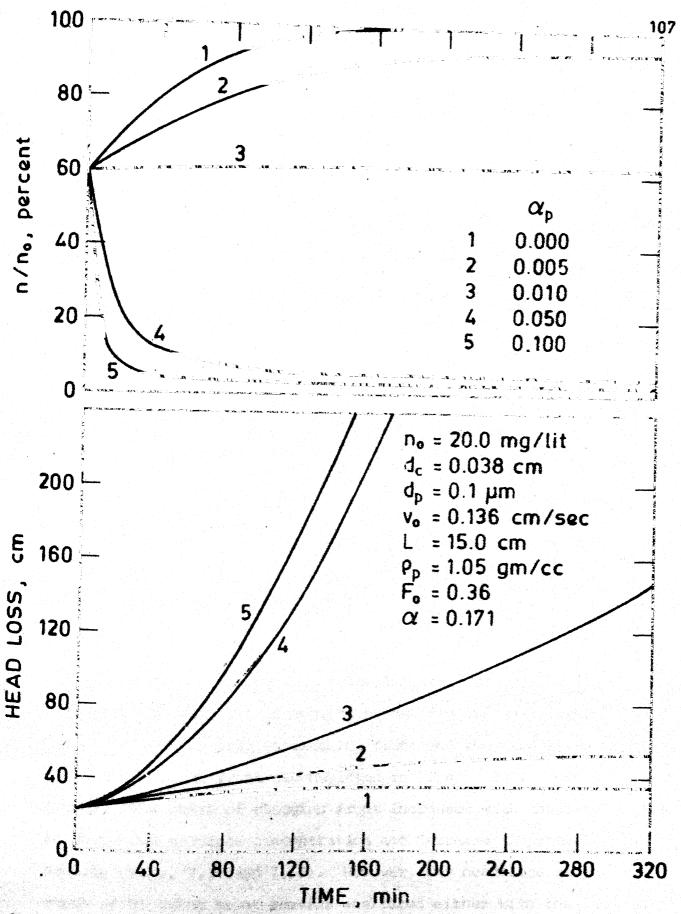


Fig. 7.10. Influence of particle-to-particle attachment on filter performance.

(Crapps, 1964; Hudson, 1964; Adin and Rebhun, 1974). However, the theoretical formulation to obtain the clogging front is not yet available.

The clogging front is defined by the points where the head loss gradient begins to deviate significantly from the value for a clean filter bed. Mathematically the clogging front may be defined by the locus of the point where the rate of change of the head loss gradient becomes zero, and may be expressed by the following equation.

$$\frac{d}{dL} (dh_f/dL) = 0 (7.1)$$

or

$$\frac{d^2}{dL^2} (h_f) = 0 (7.2)$$

Thus using Eqs. (4.7) and (7.2) the dynamic behaviour of the clogging front which would indirectly define the filter state can be predicted. The simulation of the dynamics of the clogging front for various physical and physico-chemical parameters is described as follows.

A. Physical Properties of the Influent Suspension: Influence of suspended particle concentration, density and size on the variation of the depth of clogging front and the head loss at the depth of clogging front are depicted in Figs. 7.11 to 7.13 respectively. The depth of clogging front increases with the increase in suspended particle concentration and decrease in particle density (Figs. 7.11 and 7.12). However, the head loss at the depth of clogging front remains unaltered either with the variation

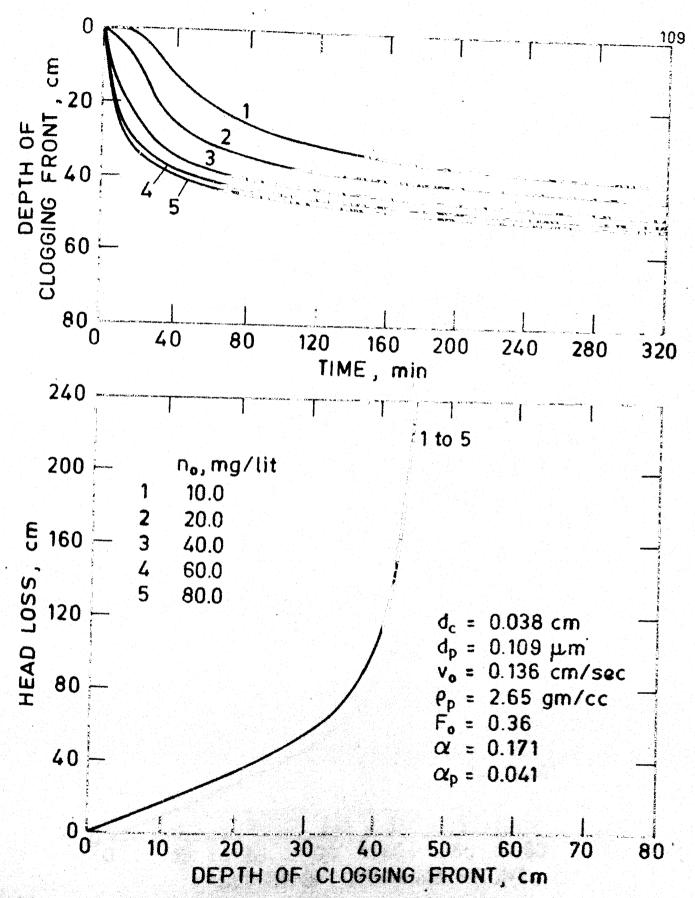


Fig. 7.11. Effect of suspended particle concentration on temporal variation of the depth of clogging front and its relationship with head loss.

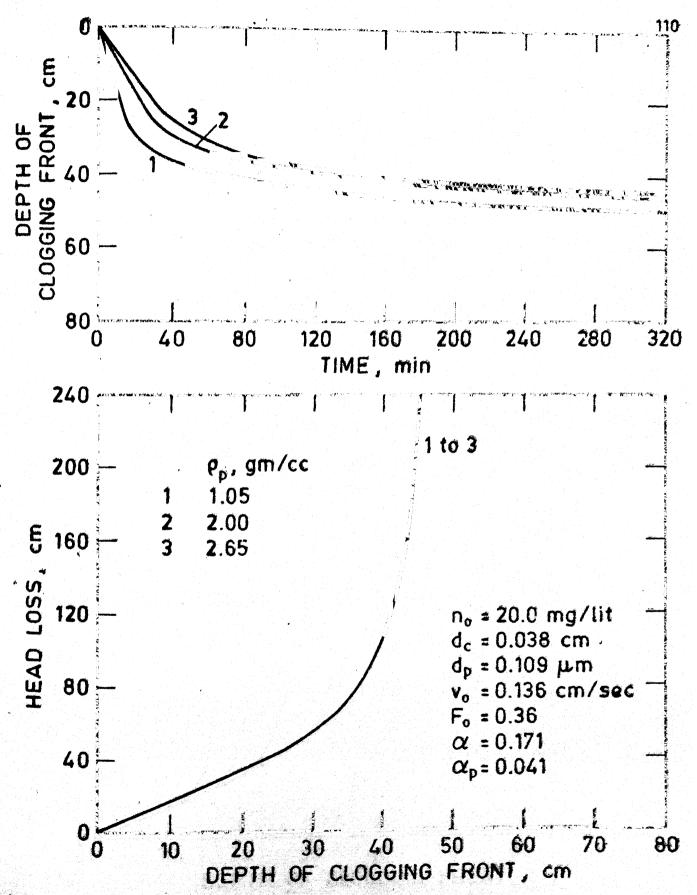


Fig. 7.12. Effect of suspended particle density on temporal variation of the depth of clogging front and its relationship with head loss.

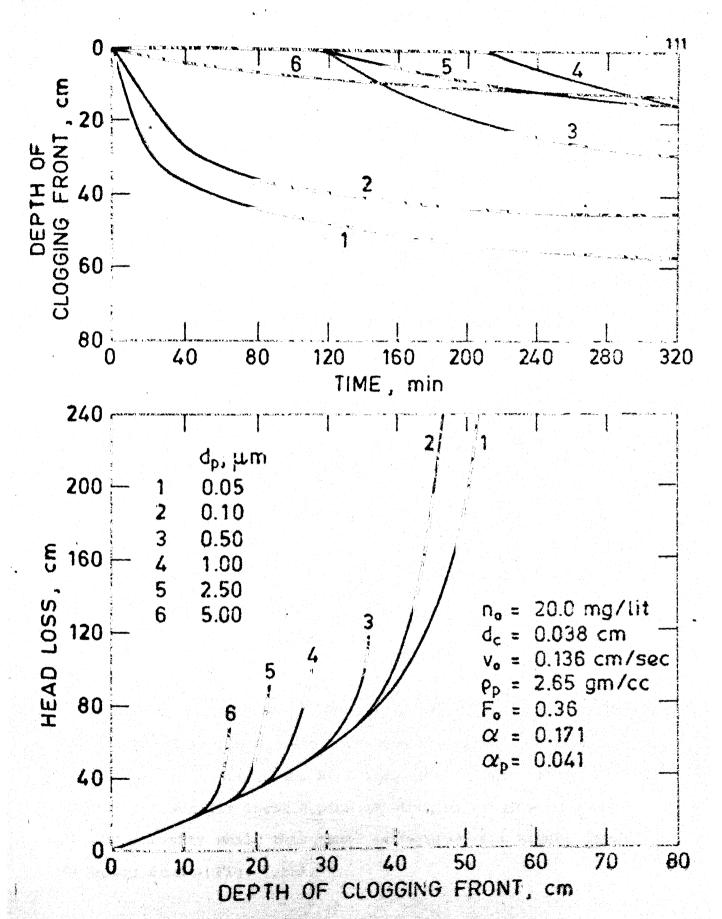


Fig. 7.13. Effect of suspended particle size on temporal variation of clogging front and its relationship with head lass.

in suspended particle concentration or density. Here again the suspended particle size show a typical behaviour. One micron particles take the longest time to form a noticeable clogging zone. Submicron particles form a deeper clogging zone from the beginning of the filtration process. The larger particles also form the clogging zone from the beginning but the depth is very very small.

- B. Media Size: Media size plays an important role in the penetration of the flocs. As the media size increases the depth of floc penetration increases. Further the head loss build-up at the depth of clogging front is lower for higher media sizes (Fig. 7.14). The size of the media can be controlled very easily and hence depending upon the input conditions $(n_0, \rho_p, d_p, \alpha,$ and $\alpha_p)$ the appropriate media size can be choosen to achieve the required filtrate quality and more uniform distribution of the particle by predicting the filter performance and the nature of clogging front using the proposed model.
- C. Clean Bed Porosity: The variation of the depth of clogging front and head loss at the depth of clogging front for four different initial bed porosities are plotted in Fig. 7.15. The depth of floc penetration increases with the decrease in initial bed porosity. The head loss at the depth of clogging front is lower for lower depths of clogging front with increase in bed porosity while this trend is reversed for higher depths of clogging front (Fig. 7.15).

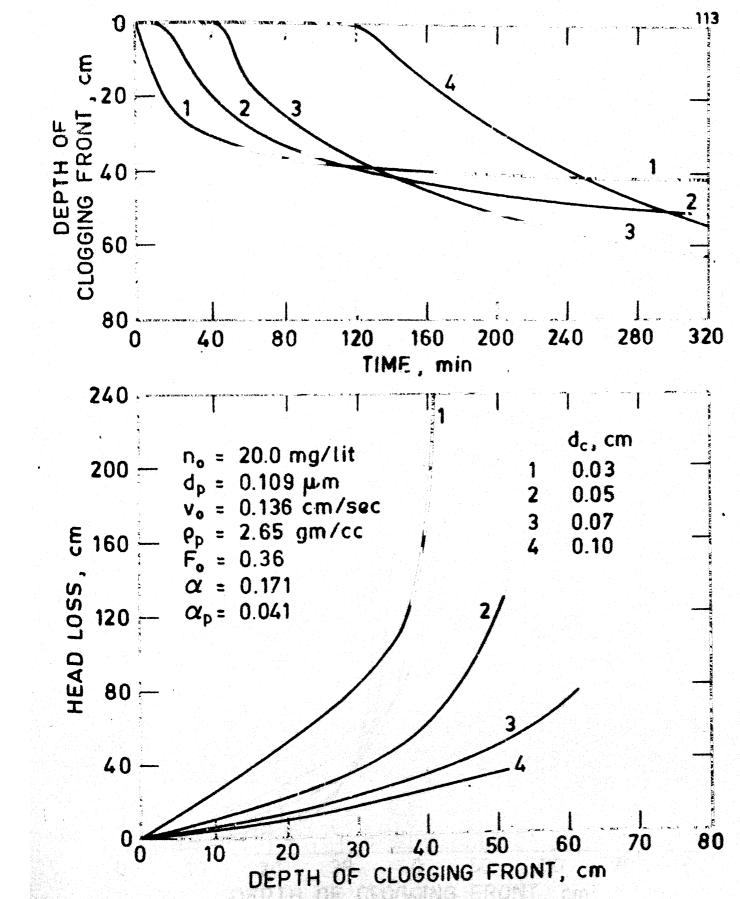


Fig. 7.14 Effect of filter media size on temporal variation of the depth of clogging front and its relationship with head loss.

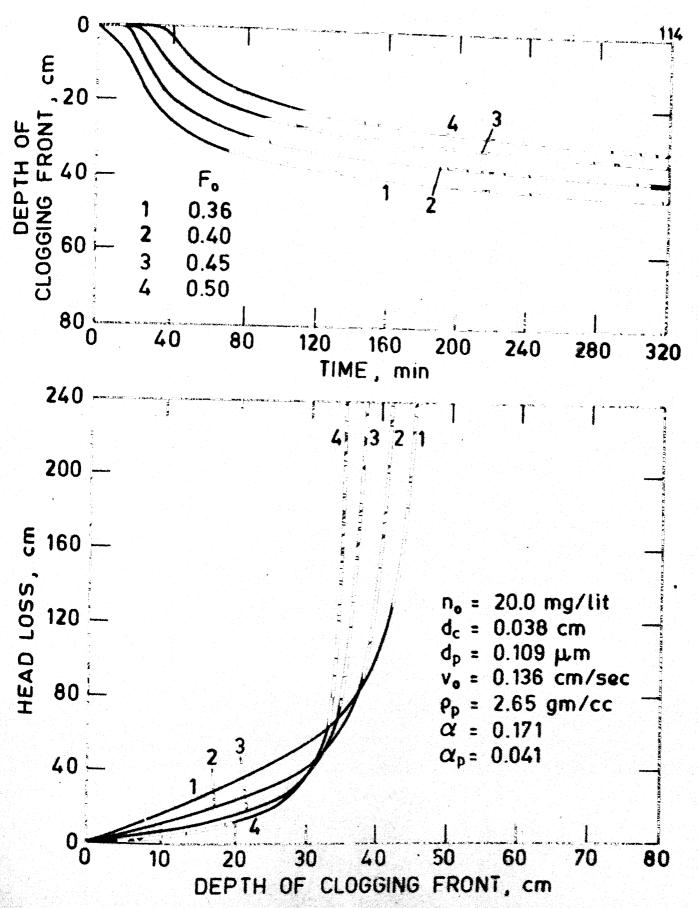


Fig. 7.15. Effect of initial bed porosity on temporal variation of the depth of clogging front and its relationship with head loss.

- D. Flow Rate: As expected the depth of clogging front increases with the increase in flow rate (Fig. 7.16). However, the head loss built at the depth of clogging front follows a very typical trend. For lower depths of clogging front the head loss is higher with higher flow rates whereas at higher depths of clogging front the head loss is higher with lower flow rates. This clearly indicates that with higher flow rates the deposition is more uniform.
- meters are represented by particle-to-media grain attachment and particle-to-particle attachment. The variation in the depth of clogging front and its relationship with head loss for physico-chemical parameters may be studied by varying the coefficients α and $\alpha_{\rm p}$ in the proposed model. The simulation results are presented in Figs. 7.17 and 7.18. The particle-to-media grain attachment does not have much significance with respect to the depth of floc penetration. The control of particle-to-particle attachment to some extent can distribute the removal over the depth of the filter bed. The head loss at the depth of clogging front is ofcourse a direct consequence of the amount of deposited material and in general has no relation with either α or $\alpha_{\rm p}$.

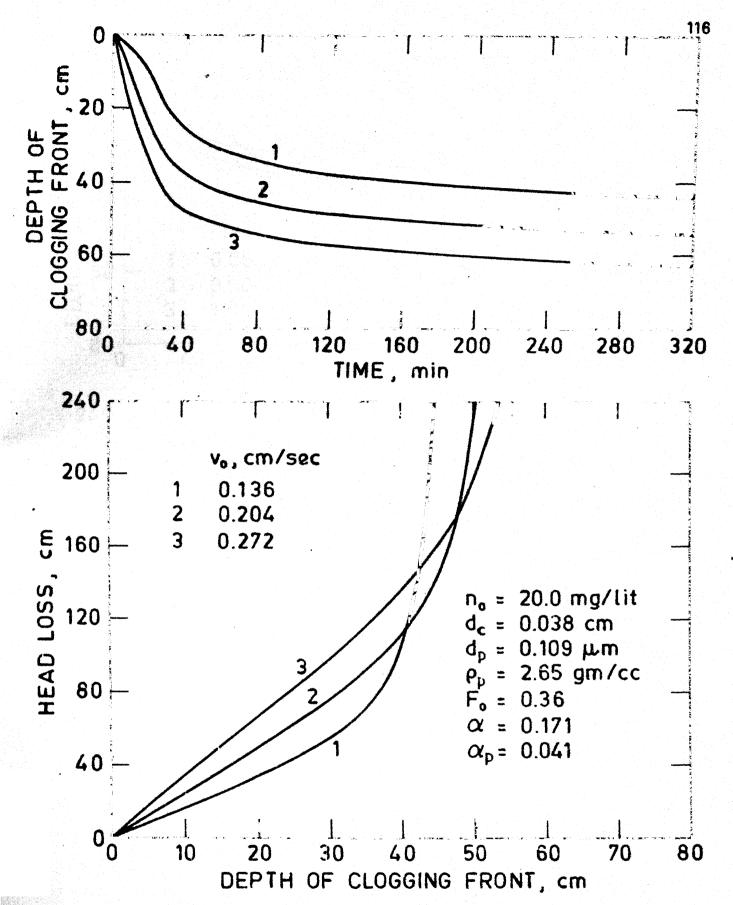


Fig. 7.16. Effect of filtration rate on temporal variation of the depth of clogging front and its relationship with head loss.

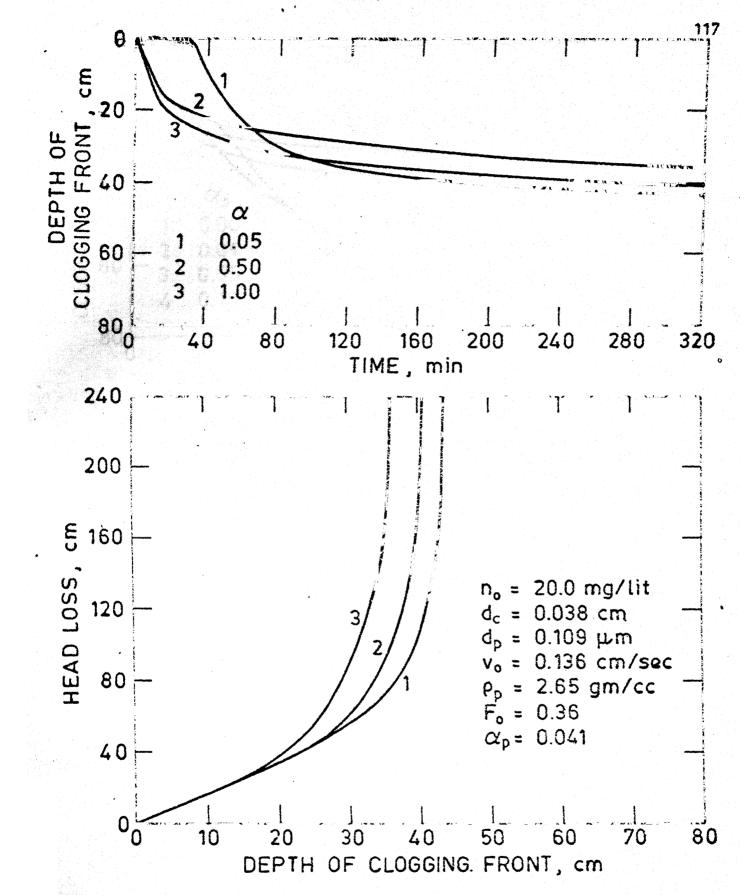


Fig. 7.17. Effect of particle-to-filter grain attachment on temporal variation of the depth of clogging front and its relationship with head loss.

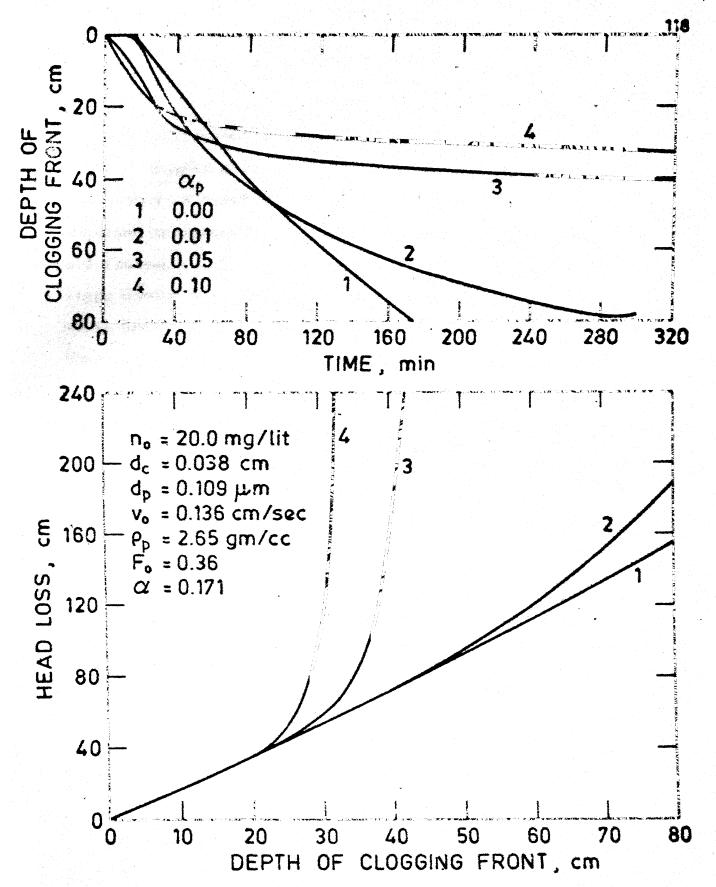


Fig. 7.18. Effect of particle-to-particle attachment on temporal variation of the depth of clogging front and its relationship with head loss.

8. SUMMARY

In the present study a simulation procedure is developed for the dynamic prediction of filter performance and filter state. The method is based on synthesizing available quantitative results relating to filtration and to porous media flows, within an overall framework which views the process to consist of two principle steps namely the transport of the suspended particles to filter media grains or already retained particles and the attachment of these particles to the filter media grain or retained particles acting as collectors. Evaluation of the results through comparison with the data available in literature and the data obtained in the experimental investigation of the present study indicates, to the extent the nature of these types of data permits, that the method is very effective and even capable of predicting on satisfactorily quantitative basis some intricate details of observed filter behaviour.

In the simulation procedure, the filter performance is characterized by the filtrate quality and the head loss development. The filter state is defined by the depth of the clogging front which decides the clogging zone in the filter bed. The results of the simulation studies indicate that the proposed model is able to predict the filter performance in accordance with the observations made in laboratory and field. Based on the results of the simulation studies following significant observations are made which may lead to the process modification and/or development of suitable design criteria for the deep bed filters.

The major important input parameters which affect the filter performance are the size of the suspended particles and their distribution. As the suspended particle size decreases the head loss development increases for the same amount of removal. The filtration efficiency though influenced by particle size, a generalized statement regarding the variation of filter efficiency with particle size is not possible because it is affected by both transport and attachment step. The transport efficiency is minimum for suspended particles around one micron while the attachment efficiency is expected to increase with the increase in particle size. The overall removal efficiency depends upon the resultant effect of both transport and attachment step.

The another important input parameter is the density of the suspended particle which controlles the number of particles in the suspension if the filter influent concentration is expressed in terms of mass per unit volume. To be very precise the filter load should be expressed in terms of the number of particles per unit volume with particle size distribution rather than expressing the same in mass per unit volume or turbidity units.

There are several other system and operating variables which influence the filter performance whose effect can very well be studied from the proposed model and can be manipulated in the actual practice to get the optimum output conditions with respect to filtrate quality and head loss development. The depth of clogging front may be used as a criteria for the design of filter depth.

9. RECOMMENDATIONS FOR FUTURE RESEARCH

On the basis of the results of the current investigation the following recommendations are made for the future research as a logical continuation of the research presented in this thesis.

- 1. The proposed model should be verified for varying suspended particle sizes in the filter influent.
- 2. The simulation model should be modified to incorporate the possible reentrainment of the deposited particles.
- 3. The possible changes in the size of the suspended particle within the pores of the filter bed because of coagulation should be predicted and appropriately incorporated in the simulation model.
- 4. The model should be extended to include the effect of irregular shapes of the suspended particles and the media grains.
- 5. A better understanding of the influence of physico-chemical parameters on filtration is necessary. This may be done utilizing the knowledge of coagulation and stating the similarities between coagulation and filtration. A model should be formulated relating α and α_p to surface characteristics (zeta potentials) of the media grains and suspended particles. This warrents detailed experimental investigation on coagulation and filtration with the proper control of the surface properties, in particular surface potentials of the media and suspended particles.

The aforementioned improvements, however, cannot be made with further experiments performed under well defined conditions. The importance of data gathered from a systematic programme of critical experiments is self-evident.

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APPENDIX A

SOLUTION TECHNIQUE

Equations (4.2), (4.3), and (4.4) constitute the mathematical model for predicting the filter effluent quality.

These equations can be rewritten as

$$\eta_{\mathbf{r}} = \eta \alpha \left(d_{\mathbf{c}}^{2} - \beta_{\mathbf{c}} \, N \, d_{\mathbf{p}}^{2} \right) / d_{\mathbf{c}}^{2} + \beta_{\mathbf{c}} \, N \, \eta \alpha_{\mathbf{p}} \left(d_{\mathbf{p}} / d_{\mathbf{c}} \right)^{2} \\
+ \left(1 - \beta_{\mathbf{c}} \right) \, N \, \eta_{\mathbf{p}} \, \alpha_{\mathbf{p}} \left(\frac{d_{\mathbf{p}}}{d_{\mathbf{c}}} \right)^{2} \tag{A.1}$$

$$\frac{\partial N}{\partial t} + V_0 \frac{\partial N}{\partial L} = \left[C_1 + N(C_3 - \beta_C C_3) - N^2 C_4\right] n \qquad (A.2)$$

$$\frac{\partial n}{\partial t} + V_0 \frac{\partial n}{\partial L} + \frac{3}{2} \frac{(1 - F)}{\partial c} V_0 n \eta_r = 0$$
 (A.3)

The analytical solution of the above equations is not possible. Therefore, simplifying techniques are used to obtain a reasonably accurate solution. The algorithm to solve these equation proceeds as follows.

Considering n and N as step functions of time and length instead of continuous ones, Eq. (A.1) for the i^{th} time interval and j^{th} length element may be written as

$$\eta_{\mathbf{r}_{\mathbf{j},\mathbf{i}}} = \eta \alpha \left(d_{\mathbf{c}}^{2} - \beta_{\mathbf{c}} N_{\mathbf{j},\mathbf{i}} d_{\mathbf{p}}^{2} \right) / d_{\mathbf{c}}^{2} + \beta_{\mathbf{c}} N_{\mathbf{j},\mathbf{i}} \eta \alpha_{\mathbf{p}} \left(\frac{d_{\mathbf{p}}}{d_{\mathbf{c}}} \right)^{2}$$

$$+ (1 - \beta_{\mathbf{c}}) N_{\mathbf{j},\mathbf{i}} \eta_{\mathbf{p}} \alpha_{\mathbf{p}} \left(\frac{d_{\mathbf{p}}}{d_{\mathbf{c}}} \right)^{2} \qquad (A.4)$$

with the boundary condition

$$N_{1,1}$$
 to $N_{\rm NL,1}$ = 0 resulting in $\eta_{\rm r_{1,1}}$ to $\eta_{\rm r_{\rm NL,1}}$ = $\eta\alpha$

Here, NL is the total number of length elements.

Assuming n to remain constant for a very small time interval Δt , Eq. (A.3) for the ith time interval reduces to

$$v_{o \ \partial L}^{\partial \dot{n}} i + \frac{3}{2} \frac{(1 - F)}{\dot{d}_{c}} v_{o \ \dot{n}_{i}} \eta_{r_{i}} = 0$$
 (A.5)

The above equation for the jth length element may be written as

$$\Delta n_{j,i} = -\frac{3}{2} \frac{(1-F)}{d_c} n_{j,i} \eta_{r_{j,i}} . \Delta L$$
 (A.5)

Here, AL is the thickness of the jth element. Further one may write

$$n_{\mathbf{j}+1,\mathbf{i}} = n_{\mathbf{j},\mathbf{i}} + \Delta n_{\mathbf{j},\mathbf{i}}$$
 (A.6)

with the boundary condition

$$n_{1.1}$$
 to $n_{1,NT} = n_0$

Here, NT is the total number of time intervals.

Similarly, Eq. (A.2) for the ith time interval and jth length step may be written as

$$\Delta N_{j,i} = [C_1 + N_{j,i} (C_3 - \beta_C C_3) - N_{j,i}^2 C_4] n_{j,i} (A.7)$$

and

$$N_{j,i+1} = N_{j,i} + \Delta N_{j,i}$$
 (A.8)

with the initial boundary condition

$$N_{1,i}$$
 to $N_{1,NL} = 0.0$

A flow sheet illustrating the above procedure is given in Fig. A.1.

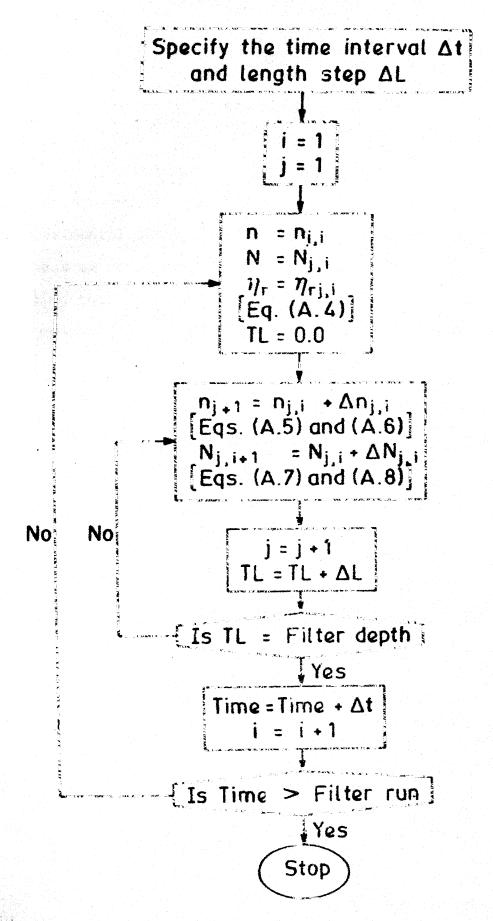


Fig. A.1. Proposed (ALGORITHM) logic diagram for predicting filtrate quality.

The procedure used was proposed by Marquardt (1963) as an extension of the Gauss Newton method to allow for convergence with relatively poor starting guesses for the unknwon coefficients. In this method, the Gauss Newton normal equations are modified by adding a factor λ ,

$$[\underline{\mathbf{A}}^{t}\underline{\mathbf{A}} + \lambda \cdot \mathbf{I}] \Delta \hat{\mathbf{A}} = \underline{\mathbf{A}}^{t} (\underline{\mathbf{y}} - \hat{\mathbf{y}}^{*})$$
 (B.3)

Here,

$$\frac{\partial}{\partial \hat{\mathbf{1}}} = \frac{\partial \hat{\mathbf{Y}}_{1}}{\partial \hat{\mathbf{A}}_{1}} = \frac{\partial \hat{\mathbf{Y}}_{1}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{2}}{\partial \hat{\mathbf{A}}_{1}} = \frac{\partial \hat{\mathbf{Y}}_{2}}{\partial \hat{\mathbf{A}}_{1}} = \frac{\partial \hat{\mathbf{Y}}_{2}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{2}}{\partial \hat{\mathbf{A}}_{1}} = \frac{\partial \hat{\mathbf{Y}}_{1}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{2}}{\partial \hat{\mathbf{A}}_{1}} = \frac{\partial \hat{\mathbf{Y}}_{2}}{\partial \hat{\mathbf{A}}_{1}} = \frac{\partial \hat{\mathbf{Y}}_{1}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{2}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{2}}{\partial \hat{\mathbf{A}}_{1}} = \frac{\partial \hat{\mathbf{Y}}_{1}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{2}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{1}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{2}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{1}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{1}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{2}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{1}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{2}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{1}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{2}}{\partial \hat{\mathbf{A}}_{2}} = \frac{\partial \hat{\mathbf{Y}}_{2}}{\partial$$

I is the identity matrix, \mathbf{A}^{t} is the transpose of \mathbf{A} matrix, and the asterisk designates quantities evaluated at the initial trial values.

Thus λ is added to each term of the main diagonal of the A^{t} A matrix. The rules for calculating λ are discussed in the original article by Marquardt (1963). All other computational details parallel - the Gauss Newton procedure.

The computer programme utilizing aforementioned algorithm is available in "Optimization Techniques with Fortran" (Kuester and Mize, 1973). The programme consists of a main programme, a general subroutine BSCLVE, a general function subprogramme ARCOSS, and two user supplied subroutines, FUNC and DERIV.
All input and output is through the main programme.

APP ENDIX C

STATISTICAL PARAMETERS

The two important statistical parameters which are generally used to check the accuracy of the models are

- (1) Coefficient of Correlation
- (2) Standard Error of Estimate

Though the coefficient of correlation has limited applicability in the nonlinear case (Tukey, 1977) it was used only for comparative purposes along with means and Standard Error of Estimate.

(1) Expression for coefficient of correlation (R):

$$R = \begin{cases} \sum_{i=1}^{n} x_i y_i - n \overline{x} \overline{y} \\ s_x s_y & \overline{n-1} \end{cases}$$
 (C.1)

Here.

$$S_{x} = \begin{cases} \sum_{i=1}^{n} (x_{i} - \bar{x})^{2} \\ \sum_{i=1}^{n} (x_{i} - \bar{x})^{2} \\ \sum_{i=1}^{n} (y_{i} - \bar{y}) \\ \sum_{i=1}^{n} (y_{i} - \bar{y}) \end{cases}$$

 $x_i = i^{th}$ experimental value,

Y_i = ith model predicted value,

 \bar{x} = average of the observed values,

 \overline{Y} = average of the model predicted values, and

n = total number of observations.

(2) Expression for standard error of estimate (5):

(C.2)

Here,

 $x_i = i^{th}$ experimental value,

 $Y_i = i^{th}$ model predicted value,

n = total number of observations, and

K = number of unknowns.